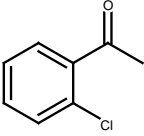
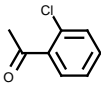


Query

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Reaxys ID 1858916 View in Reaxys		1/1
		<p>CAS Registry Number: 2142-68-9 Chemical Name: 1-(2-chlorophenyl)ethan-1-one; o-chlorophenyl methyl ketone; 1-(2-chlorophenyl)ethanone; 2'-chloroacetophenone; o-Chloroacetophenone; o-Cl(C₆H₄)COMe; 1-(2-chloro-phenyl)-ethanone Linear Structure Formula: Cl(C₆H₄)C(O)CH₃ Molecular Formula: C₈H₇ClO Molecular Weight: 154.596 Type of Substance: isocyclic InChI Key: ZDOYHCIRUPHUHN-UHFFFAOYSA-N Note:</p>
Substance Label (132)		
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1.5498	587.6	16.6	v. Auwers; Lechner; Bundesmann ; Chemische Berichte; vol. 58; (1925); p. 48, View in Reaxys
1.5631	486.1	16.6	v. Auwers; Lechner; Bundesmann ; Chemische Berichte; vol. 58; (1925); p. 48, View in Reaxys
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Density (4)			
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	Reference Temperature [°C]	4	
	Measurement Temperature [°C]	30	
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2 of 4	Density [gcm-3]	1.18	

	Reference Temperature [°C]	4
	Measurement Temperature [°C]	30
Baliah; Aparajithan ; Tetrahedron; vol. 19 ; (1963); p. 2177,2183, View in Reaxys		
3 of 4	Density [gcm-3]	1.2016
	Reference Temperature [°C]	4
	Measurement Temperature [°C]	16.6
v. Auwers; Lechner; Bundesmann ; Chemische Berichte; vol. 58 ; (1925); p. 48, View in Reaxys		
4 of 4	Density [gcm-3]	1.1884
	Reference Temperature [°C]	25
	Measurement Temperature [°C]	25
Thorp; Brunskill ; Journal of the American Chemical Society; vol. 37 ; (1915); p. 1262, View in Reaxys		
Chromatographic Data (1)		
Chromatographic data	Location	References
GC (Gas chromatography)	supporting information	Johnson, Tarn C.; Totty, William G.; Wills, Martin ; Organic Letters; vol. 14 ; nb. 20; (2012); p. 5230 - 5233, View in Reaxys ; Wang, Rui; Wan, Jingwei; Ma, Xuebing; Xu, Xiao; Liu, Liu ; Dalton Transactions; vol. 42 ; nb. 18; (2013); p. 6513 - 6522, View in Reaxys ; Goek, Luetfiye; Tuerkmen, Hayati ; Tetrahedron; vol. 69 ; nb. 49; (2013); p. 10669 - 10674, View in Reaxys ; Ganesamoorthy; Muthu Tamizh; Shanmugasundaram; Karvembu ; Tetrahedron Letters; vol. 54 ; nb. 51; (2013); p. 7035 - 7039, View in Reaxys ; Li, Min; Li, Bin; Xia, Hong-Feng; Ye, Danru; Wu, Jing; Shi, Yifeng ; Green Chemistry; vol. 16 ; nb. 5; (2014); p. 2680 - 2688, View in Reaxys ; Paul, Caroline E.; Rodriguez-Mata, Maria; Busto, Eduardo; Lavandera, Ivan; Gotor-Fernandez, Vicente; Gotor, Vicente; Garcia-Cerrada, Susana; Mendiola, Javier; De Frutos, Oscar; Collado, Ivan ; Organic Process Research and Development; vol. 18 ; nb. 6; (2014); p. 788 - 792, View in Reaxys
Conformation (1)		
Object of Investigation	References	
Conformation	Forbes ; Canadian Journal of Chemistry; vol. 38 ; (1960); p. 1104,1107, View in Reaxys ; Baliah; Aparajithan ; Tetrahedron; vol. 19 ; (1963); p. 2177,2183, View in Reaxys ; Mirarchi, D.; Ritchie, G. L. D. ; Journal of Molecular Structure; vol. 118 ; (1984); p. 303 - 310, View in Reaxys	
Crystal Property Description (6)		
Colour & Other Properties	Location	References
colourless		Shi, Xiang-Jun; Qian, Jie; Tan, Fan-Fan; Yu, Chuan-Ming ; Journal of Chemical Research; vol. 37 ; nb. 7; (2013); p. 398 - 401, View in Reaxys ; Xie, Aming; Zhou, Xiangxiang; Feng, Liandong; Hu, Xinyu; Dong, Wei ; Tetrahedron; vol. 70 ; nb. 21; (2014); p. 3514 - 3519, View in Reaxys
yellow	supporting information	Wang, Yu-Fei; Gao, Ya-Ru; Mao, Shuai; Zhang, Yan-Lei; Guo, Dong-Dong; Yan, Zhao-Lei; Guo, Shi-Huan; Wang, Yong-Qiang ; Organic Letters; vol. 16 ; nb. 6; (2014); p. 1610 - 1613, View in Reaxys
white		Moriyama, Katsuhiko; Takemura, Misato; Togo, Hideo ; Journal of Organic Chemistry; vol. 79 ; nb. 13; (2014); p. 6094 - 6104, View in Reaxys
white	supporting information	Moriyama, Katsuhiko; Nakamura, Yu; Togo, Hideo ; Organic Letters; vol. 16 ; nb. 14; (2014); p. 3812 - 3815, View in Reaxys
yellow		Zhang, Jinli; Han, Zixing; Li, Junmiao; Wu, Yangjie ; Arkivoc; vol. 2013 ; nb. 4; (2013); p. 251 - 271, View in Reaxys
colourless		Wang, Lian-Yue; Li, Jun; Lv, Ying; Zhang, Heng-Yun; Gao, Shuang ; Journal of Organometallic Chemistry; vol. 696 ; nb. 20; (2011); p. 3257 - 3263, View in Reaxys
Dielectric Constant (1)		

References	
Sorriso; Foffani ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1973); p. 1497, View in Reaxys	
Electrical Data (2)	
1 of 2	Description Dielectric relaxation time Klages; Knobloch ; Zeitschrift fuer Naturforschung, Teil A: Astrophysik, Physik und Physikalische Chemie; vol. 20; (1965); p. 580,582, View in Reaxys ; Mitra; Ghosh; Acharyya ; Journal of the Indian Chemical Society; vol. 83; nb. 12; (2006); p. 1230 - 1235, View in Reaxys
2 of 2	Description Dielectric loss Klages; Knobloch ; Zeitschrift fuer Naturforschung, Teil A: Astrophysik, Physik und Physikalische Chemie; vol. 20; (1965); p. 580,582, View in Reaxys
Electrical Moment (6)	
1 of 6	Description Dipole moment Moment [D] 1.94264 - 2.04757 Temperature [°C] 30 - 45 Method Dielectric constant (ϵ) Solvent benzene Mitra; Ghosh; Acharyya ; Journal of the Indian Chemical Society; vol. 83; nb. 12; (2006); p. 1230 - 1235, View in Reaxys
2 of 6	Description Dipole moment Comment Tab. 1; Dipolmoment exp., ber. Tab. 2 Sorriso; Foffani ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1973); p. 1497, View in Reaxys
3 of 6	Description Dipole moment Comment μ Cheng et al. ; Journal of the Chemical Society [Section] B: Physical Organic; (1971); p. 1198, View in Reaxys
4 of 6	Description Dipole moment Klages; Knobloch ; Zeitschrift fuer Naturforschung, Teil A: Astrophysik, Physik und Physikalische Chemie; vol. 20; (1965); p. 580,582, View in Reaxys
5 of 6	Description Dipole moment Comment 3.15 D (E, Bzl., 30grad) Baliah; Aparajithan ; Tetrahedron; vol. 19; (1963); p. 2177,2183, View in Reaxys
6 of 6	Description Dipole moment Comment 3.21 D (E, Bzl., 50grad) Baliah; Aparajithan ; Tetrahedron; vol. 19; (1963); p. 2177,2183, View in Reaxys
Electrochemical Characteristics (2)	
1 of 2	Description polarographic half-wave potential Jones; Rowlinson ; Journal of Electroanalytical Chemistry and Interfacial Electrochemistry; vol. 19; (1968); p. 297,299, View in Reaxys
2 of 2	Description polarographic half-wave potential Comment (wss. Dioxan vom pH 0). Coulson et al. ; Journal of the American Chemical Society; vol. 79; (1957); p. 1354,1355, View in Reaxys
Further Information (3)	
Description	References
Further information	Jones; Rowlinson ; Journal of Electroanalytical Chemistry and Interfacial Electrochemistry; vol. 19; (1968); p. 297,299, View in Reaxys
Further information	Gupta; Mital ; Bulletin des Societes Chimiques Belges; vol. 76; (1967); p. 631,634, 636, View in Reaxys

Further information	Dhami; Stothers ; Tetrahedron Letters; (1964); p. 631,634, View in Reaxys	
Magnetic Susceptibility (1)		
References		
Goyal et al. ; Indian Journal of Chemistry; vol. 9 ; (1971); p. 696, View in Reaxys		
Optics (1)		
Description	References	
Electric birefringence (Kerr effect)	Cheng et al. ; Journal of the Chemical Society [Section] B: Physical Organic; (1971); p. 1198, View in Reaxys ; Mirarchi, D.; Ritchie, G. L. D. ; Journal of Molecular Structure; vol. 118 ; (1984); p. 303 - 310, View in Reaxys	
Sound Properties (1)		
Description	References	
Ultrasonic properties	Pethrick; Wyn-Jones ; Transactions of the Faraday Society; vol. 66 ; (1970); p. 2483,2485, View in Reaxys	
Static Dielectric Constant (1)		
Static Dielectric Constant	Temperature [°C]	References
14	30	Ponomarenko, S. P.; Nikalaenko, T. K.; Makovetskii, V. P.; Borovikov, Yu. Ya.; Kukhar, V. P. ; Russian Journal of General Chemistry; vol. 64 ; nb. 5.2; (1994); p. 735 - 739; Zhurnal Obshchei Khimii; vol. 64 ; nb. 5; (1994); p. 812 - 817, View in Reaxys
NMR Spectroscopy (25)		
1 of 25	Description	Chemical shifts; Spectrum
	Nucleus	¹³ C
	Solvents	chloroform-d1
	Frequency [MHz]	100
	Location	supporting information
	Li, Xiao-Qiang; Wang, Wei-Kun; Han, Yi-Xin; Zhang, Chi ; Advanced Synthesis and Catalysis; vol. 352 ; nb. 14-15; (2010); p. 2588 - 2598, View in Reaxys ; Wang, Yu-Fei; Gao, Ya-Ru; Mao, Shuai; Zhang, Yan-Lei; Guo, Dong-Dong; Yan, Zhao-Lei; Guo, Shi-Huan; Wang, Yong-Qiang ; Organic Letters; vol. 16 ; nb. 6; (2014); p. 1610 - 1613, View in Reaxys	
2 of 25	Description	Chemical shifts; Spectrum
	Nucleus	¹ H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	Location	supporting information
	Wang, Yu-Fei; Gao, Ya-Ru; Mao, Shuai; Zhang, Yan-Lei; Guo, Dong-Dong; Yan, Zhao-Lei; Guo, Shi-Huan; Wang, Yong-Qiang ; Organic Letters; vol. 16 ; nb. 6; (2014); p. 1610 - 1613, View in Reaxys ; Moriyama, Katsuhiko; Takemura, Misato; Togo, Hideo ; Journal of Organic Chemistry; vol. 79 ; nb. 13; (2014); p. 6094 - 6104, View in Reaxys ; Moriyama, Katsuhiko; Nakamura, Yu; Togo, Hideo ; Organic Letters; vol. 16 ; nb. 14; (2014); p. 3812 - 3815, View in Reaxys	
3 of 25	Description	Chemical shifts; Spectrum
	Nucleus	¹ H
	Solvents	chloroform-d1
	Frequency [MHz]	300
	Original Text	¹ H NMR (300 MHz, CDCl ₃) δ 7.54 (m, 1H), 7.40 (m, 2H), 7.35 (m, 1H), 2.65 (s, 3H)
	Location	supporting information
	Signals [ppm]	7.54; 7.4; 7.35; 2.65
	Kind of signal	m, 1H; m, 2H; m, 1H; s, 3H
	Xie, Aming; Zhou, Xiangxiang; Feng, Liandong; Hu, Xinyu; Dong, Wei ; Tetrahedron; vol. 70 ; nb. 21; (2014); p. 3514 - 3519, View in Reaxys	
4 of 25	Description	Chemical shifts; Spectrum

	Nucleus	13C
	Solvents	chloroform-d1
	Frequency [MHz]	75
	Original Text	¹³ C NMR (75 MHz, CDCl ₃) δ 200.37, 139.01, 131.93, 131.17, 130.56, 129.32, 126.86, 30.63
	Location	supporting information
	Signals [ppm]	200.37; 139.01; 131.93; 131.17; 130.56; 129.32; 126.86; 30.63
	Xie, Aming; Zhou, Xiangxiang; Feng, Liandong; Hu, Xinyu; Dong, Wei; Tetrahedron; vol. 70; nb. 21; (2014); p. 3514 - 3519, View in Reaxys	
5 of 25	Description	Chemical shifts; Spectrum
	Nucleus	13C
	Solvents	chloroform-d1
	Frequency [MHz]	100
	Location	supporting information
	Moriyama, Katsuhiko; Takemura, Misato; Togo, Hideo; Journal of Organic Chemistry; vol. 79; nb. 13; (2014); p. 6094 - 6104, View in Reaxys ; Moriyama, Katsuhiko; Nakamura, Yu; Togo, Hideo; Organic Letters; vol. 16; nb. 14; (2014); p. 3812 - 3815, View in Reaxys	
6 of 25	Description	Chemical shifts
	Nucleus	13C
	Solvents	chloroform-d1
	Frequency [MHz]	100
	Li, Xiao-Qiang; Wang, Wei-Kun; Zhang, Chi; Advanced Synthesis and Catalysis; vol. 351; nb. 14-15; (2009); p. 2342 - 2350, View in Reaxys ; Zhang, Jinli; Han, Zixing; Li, Junmiao; Wu, Yangjie; Arkivoc; vol. 2013; nb. 4; (2013); p. 251 - 271, View in Reaxys	
7 of 25	Description	Chemical shifts; Spectrum
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	Location	supporting information
	Li, Xiao-Qiang; Wang, Wei-Kun; Han, Yi-Xin; Zhang, Chi; Advanced Synthesis and Catalysis; vol. 352; nb. 14-15; (2010); p. 2588 - 2598, View in Reaxys ; Ganesamoorthy; Muthu Tamizh; Shanmugasundaram; Karvembu; Tetrahedron Letters; vol. 54; nb. 51; (2013); p. 7035 - 7039, View in Reaxys	
8 of 25	Description	Chemical shifts; Spectrum
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	500
	Location	supporting information
	Zhang, Guofu; Xie, Xiaoqiang; Wang, Yong; Wen, Xin; Zhao, Yun; Ding, Chengrong; Organic and Biomolecular Chemistry; vol. 11; nb. 18; (2013); p. 2947 - 2950, View in Reaxys ; Zhang, Guofu; Han, Xingwang; Luan, Yuxin; Wang, Yong; Wen, Xin; Ding, Chengrong; Chemical Communications; vol. 49; nb. 72; (2013); p. 7908 - 7910, View in Reaxys	
9 of 25	Description	Chemical shifts; Spectrum
	Nucleus	13C
	Solvents	chloroform-d1
	Frequency [MHz]	125
	Location	supporting information
	Zhang, Guofu; Xie, Xiaoqiang; Wang, Yong; Wen, Xin; Zhao, Yun; Ding, Chengrong; Organic and Biomolecular Chemistry; vol. 11; nb. 18; (2013); p. 2947 - 2950, View in Reaxys ; Zhang, Guofu; Han, Xingwang; Luan, Yuxin;	

	Wang, Yong; Wen, Xin; Ding, Chengrong ; Chemical Communications; vol. 49; nb. 72; (2013); p. 7908 - 7910, View in Reaxys	
10 of 25	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	Shi, Xiang-Jun; Qian, Jie; Tan, Fan-Fan; Yu, Chuan-Ming ; Journal of Chemical Research; vol. 37; nb. 7; (2013); p. 398 - 401, View in Reaxys ; Zhang, Jinli; Han, Zixing; Li, Junmiao; Wu, Yangjie ; Arkivoc; vol. 2013; nb. 4; (2013); p. 251 - 271, View in Reaxys	
11 of 25	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	Li, Xiao-Qiang; Wang, Wei-Kun; Zhang, Chi ; Advanced Synthesis and Catalysis; vol. 351; nb. 14-15; (2009); p. 2342 - 2350, View in Reaxys ; Wang, Lian-Yue; Li, Jun; Lv, Ying; Zhang, Heng-Yun; Gao, Shuang ; Journal of Organometallic Chemistry; vol. 696; nb. 20; (2011); p. 3257 - 3263, View in Reaxys ; Vogl, Michael; Brecker, Lothar; Kratzer, Regina; Nidetzky, Bernd ; Chirality; vol. 24; nb. 10; (2012); p. 847 - 853,7, View in Reaxys	
12 of 25	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	300
	Location	supporting information
	Cabrero-Antonino, Jose R.; Leyva-Perez, Antonio; Corma, Avelino ; Chemistry - A European Journal; vol. 18; nb. 35; (2012); p. 11107 - 11114, View in Reaxys	
13 of 25	Description	Chemical shifts
	Nucleus	13C
	Solvents	chloroform-d1
	Vogl, Michael; Brecker, Lothar; Kratzer, Regina; Nidetzky, Bernd ; Chirality; vol. 24; nb. 10; (2012); p. 847 - 853,7, View in Reaxys	
14 of 25	Description	Chemical shifts
	Nucleus	1H
	Solvents	water-d2; methanol-d4
	Temperature [°C]	27.04
	Frequency [MHz]	400.1
Vogl, Michael; Kratzer, Regina; Nidetzky, Bernd; Brecker, Lothar ; Organic and Biomolecular Chemistry; vol. 9; nb. 16; (2011); p. 5863 - 5870, View in Reaxys		
15 of 25	Description	Chemical shifts
	Nucleus	13C
	Solvents	water-d2; methanol-d4
	Temperature [°C]	27.04
	Vogl, Michael; Kratzer, Regina; Nidetzky, Bernd; Brecker, Lothar ; Organic and Biomolecular Chemistry; vol. 9; nb. 16; (2011); p. 5863 - 5870, View in Reaxys	
16 of 25	Description	Chemical shifts
	Nucleus	13C
	Solvents	chloroform-d1
	Frequency [MHz]	100.6

	Wang, Lian-Yue; Li, Jun; Lv, Ying; Zhang, Heng-Yun; Gao, Shuang; Journal of Organometallic Chemistry; vol. 696; nb. 20; (2011); p. 3257 - 3263, View in Reaxys	
17 of 25	Description	Chemical shifts
	Nucleus	¹ H
	Solvents	CDCl ₃
	Frequency [MHz]	400
	Ruan, Jiwu; Li, Xinming; Saidi, Ourida; Xiao, Jianliang; Journal of the American Chemical Society; vol. 130; nb. 8; (2008); p. 2424 - 2425, View in Reaxys	
18 of 25	Description	Chemical shifts
	Nucleus	¹³ C
	Solvents	CDCl ₃
	Frequency [MHz]	100
	Ruan, Jiwu; Li, Xinming; Saidi, Ourida; Xiao, Jianliang; Journal of the American Chemical Society; vol. 130; nb. 8; (2008); p. 2424 - 2425, View in Reaxys	
19 of 25	Description	Spectrum
	Nucleus	¹ H
	Solvents	CDCl ₃
	Frequency [MHz]	400
	Ruan, Jiwu; Li, Xinming; Saidi, Ourida; Xiao, Jianliang; Journal of the American Chemical Society; vol. 130; nb. 8; (2008); p. 2424 - 2425, View in Reaxys	
20 of 25	Description	Spectrum
	Nucleus	¹³ C
	Solvents	CDCl ₃
	Frequency [MHz]	100
	Ruan, Jiwu; Li, Xinming; Saidi, Ourida; Xiao, Jianliang; Journal of the American Chemical Society; vol. 130; nb. 8; (2008); p. 2424 - 2425, View in Reaxys	
21 of 25	Description	Chemical shifts
	Nucleus	¹ H
	Solvents	CDCl ₃
	Cai, Ming-Zhong; Song, Cai-Sheng; Huang, Xian; Journal of Chemical Research - Part S; nb. 5; (1998); p. 264 - 265, View in Reaxys	
22 of 25	Description	Chemical shifts
	Nucleus	¹³ C
	Solvents	CDCl ₃
	Sakamoto; Watanabe; Bulletin of the Chemical Society of Japan; vol. 59; nb. 10; (1986); p. 3033 - 3038, View in Reaxys ; Hoening; Magnetic Resonance in Chemistry; vol. 34; nb. 5; (1996); p. 395 - 400, View in Reaxys	
23 of 25	Description	Chemical shifts
	Nucleus	¹ H
	Kikukawa, Kiyoshi; Idemoto, Tohru; Katayama, Atsuhiko; Kono, Kiyoshi; Wada, Fumio; Matsuda, Tsutomu; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); (1987); p. 1511 - 1514, View in Reaxys	
24 of 25	Description	NMR
	Yoder et al.; Journal of Organic Chemistry; vol. 41; nb. 9; (1976); p. 1511,1512, View in Reaxys ; Bloxsidge et al.; Organic Magnetic Resonance; vol. 2; (1970); p. 337, View in Reaxys ; Cheng et al.; Journal of the Chemical Society [Section] B: Physical Organic; (1971); p. 1198, View in Reaxys ; Smith et al.; Journal of the American Chemical Society; vol. 94; (1972); p. 1959,1961, View in Reaxys	
25 of 25	Description	Chemical shifts

	Comment	13C-NMR
	Dhami, K.S.; Stothers, J.B. ; Canadian Journal of Chemistry; vol. 43 ; (1965); p. 479, View in Reaxys	
IR Spectroscopy (10)		
1 of 10	Description	ATR (attenuated total reflectance); Bands
	Solvent	neat (no solvent, solid phase)
	Moriyama, Katsuhiko; Takemura, Misato; Togo, Hideo ; Journal of Organic Chemistry; vol. 79 ; nb. 13; (2014); p. 6094 - 6104, View in Reaxys	
2 of 10	Description	Bands
	Solvent	neat (no solvent, solid phase)
	Location	supporting information
Moriyama, Katsuhiko; Nakamura, Yu; Togo, Hideo ; Organic Letters; vol. 16 ; nb. 14; (2014); p. 3812 - 3815, View in Reaxys		
3 of 10	Description	Bands
	Cheng et al. ; Journal of the Chemical Society [Section] B: Physical Organic; (1971); p. 1198, View in Reaxys ; Vogl, Michael; Kratzer, Regina; Nidetzky, Bernd; Brecker, Lothar ; Organic and Biomolecular Chemistry; vol. 9 ; nb. 16; (2011); p. 5863 - 5870, View in Reaxys	
4 of 10	Description	Bands
	Solvent	neat (no solvent)
	Ruan, Jiwu; Li, Xinming; Saidi, Ourida; Xiao, Jianliang ; Journal of the American Chemical Society; vol. 130 ; nb. 8; (2008); p. 2424 - 2425, View in Reaxys	
5 of 10	Description	Bands
	Solvent	neat (no solvent)
	Comment	3050 - 755 cm ^{**} (-1)
	Cai, Ming-Zhong; Song, Cai-Sheng; Huang, Xian ; Journal of Chemical Research - Part S; nb. 5; (1998); p. 264 - 265, View in Reaxys	
6 of 10	Description	Bands
	Solvent	neat (no solvent)
	Comment	1694 cm ^{**} (-1)
	Kolb, Vera M.; Stupar, Joseph W.; Janota, Timothy E.; Duax, William L. ; Journal of Organic Chemistry; vol. 54 ; nb. 10; (1989); p. 2341 - 2346, View in Reaxys	
7 of 10	Description	Bands
	Comment	1700 cm ^{**} (-1)
	Kikukawa, Kiyoshi; Idemoto, Tohru; Katayama, Atsuhiko; Kono, Kiyoshi; Wada, Fumio; Matsuda, Tsutomu ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); (1987); p. 1511 - 1514, View in Reaxys	
8 of 10	Description	IR
	Ghersetti et al. ; Spectroscopy Letters; vol. 8 ; (1975); p. 391,393, View in Reaxys ; Sorriso; Foffani ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1973); p. 1497, View in Reaxys	
9 of 10	Description	Spectrum
	Solvent	CCl4
	Comment	1725 - 1675 cm ^{**} (-1)
	Depireux ; Bulletin des Societes Chimiques Belges; vol. 66 ; (1957); p. 218,221, View in Reaxys	
10 of 10	Description	Intensity of IR bands
	Comment	Frequenz und Intensitaet der CO-Valenzschwingungsbande.
	Jones et al. ; Canadian Journal of Chemistry; vol. 35 ; (1957); p. 504,506, 508, 512, View in Reaxys	
Mass Spectrometry (1)		
Description	Location	References

GCMS (Gas chromatography mass spectrometry); Spectrum	supporting information	Cabrero-Antonino, Jose R.; Leyva-Perez, Antonio; Corma, Avelino; Chemistry - A European Journal; vol. 18; nb. 35; (2012); p. 11107 - 11114, View in Reaxys
UV/VIS Spectroscopy (6)		
1 of 6	Description	UV/VIS
	Seth-Paul; Vermlyen-De Winter; Journal of Molecular Structure; vol. 4; (1969); p. 303,304, View in Reaxys	
2 of 6	Description	Spectrum
	Forbes; Canadian Journal of Chemistry; vol. 38; (1960); p. 1104,1107, View in Reaxys	
3 of 6	Description	Absorption maxima
	Horton,W.J.; Robertson,D.E.; Journal of Organic Chemistry; vol. 25; (1960); p. 1016 - 1020, View in Reaxys	
4 of 6	Description	Absorption maxima
	Solvent	cyclohexane
	Absorption Maxima [nm]	235; 280
	Forbes et al.; Canadian Journal of Chemistry; vol. 35; (1957); p. 1049,1051, View in Reaxys	
5 of 6	Description	Absorption maxima
	Solvent	ethanol
	Absorption Maxima [nm]	238; 281
	Forbes; Mueller; Canadian Journal of Chemistry; vol. 35; (1957); p. 488,498, View in Reaxys ; Forbes et al.; Canadian Journal of Chemistry; vol. 35; (1957); p. 1049,1051, View in Reaxys	
6 of 6	Description	Absorption maxima
	Solvent	H2O
	Absorption Maxima [nm]	209; 243; 286
	Doub; Vandenbelt; Journal of the American Chemical Society; vol. 77; (1955); p. 4535,4539, View in Reaxys	
NQR Spectroscopy (1)		
Description	References	
Nuclear quadrupole resonance	Dewar; Herr; Tetrahedron; vol. 27; (1971); p. 2377,2378, View in Reaxys	
Luminescence Spectroscopy (2)		
Description	Comment	References
Luminescence quenching	Quenching with O2	Darmanyan, Alexander P.; Foote, Christopher S.; Journal of Physical Chemistry; vol. 96; nb. 9; (1992); p. 3723 - 3728, View in Reaxys
Luminescence lifetime		Darmanyan, Alexander P.; Foote, Christopher S.; Journal of Physical Chemistry; vol. 96; nb. 9; (1992); p. 3723 - 3728, View in Reaxys
Fluorescence Spectroscopy (1)		
Description	References	
Fluorescence lifetime	Ramseier, Markus; Senn, Paul; Wirz, Jakob; Journal of Physical Chemistry A; vol. 107; nb. 18; (2003); p. 3305 - 3315, View in Reaxys	
Pharmacological Data (11)		
1 of 11	Comment	physiological behaviour discussed
	Wang, Nengqiang; Huang, Jin; Luo, Hongdou; Wang, Pu; Li, Jun; Journal of Molecular Catalysis B: Enzymatic; vol. 92; (2013); p. 1 - 6, View in Reaxys	
2 of 11	Comment	Bioactivities present
	Rival; Grassy; Michel; Chemical and Pharmaceutical Bulletin; vol. 40; nb. 5; (1992); p. 1170 - 1176, View in Reaxys ; Summer; Klein; Lichtmannegger; Wolff; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys ; Piyachaturawat, Pawinee; Chai-Ngam, Nitjagan; Chuncharunee, Aporn; Komaratat, Prayad; Suksamrarn, Apichart; European Journal of Pharmacology; vol. 387; nb. 2; (2000); p. 221 - 227, View in Reaxys ; Zhu, Dunming; Yang, Yan; Buynak, John D.; Hua, Ling; Organic and Biomolecular Chemistry; vol. 4; nb. 14; (2006); p. 2690 - 2695, View in Reaxys ; Sivakumar, Ponnurengam Malliappan; Sheshayan, Gayathri; Doble, Mukesh; Chemical Biology and Drug Design; vol. 72; nb. 4; (2008); p. 303 - 313, View in Reaxys ; Szallasi;	

	Szolcsanyi; Blumberg; Naunyn-Schmiedeberg's archives of pharmacology; vol. 344; nb. 5; (1991); p. 551 - 556, View in Reaxys ; Patent; NISHIYAMA Tozo; YASOHARA Yoshihiko; EP1995314; (A1); (2008), View in Reaxys	
3 of 11	Effect	biotransformation
	Species or Test-System	Sporobolomyces salmonicolor carbonyl reductase AKU 4429
	Kind of Dosing	title comp. dissolved in DMSO
	Method	carbonyl reductase gene cloned and over-expressed in Escherichia coli BL21(DE3); D-glucose, D-glucose dehydrogenase, NADPH and title comp. mixed in a potassium phosphate buffer (pH 6.5) at room temp.; HPLC; specific activity determined at 340 nm
	Results	specific activity = 78 nmol*min ⁻¹ *mg ⁻¹ ; enantiomeric excess of metabolites: 15percent (R)
	Metabolite XRN	4230459; 1931619
	Metabolite	(R)-C8H9ClO; (S)-C8H9ClO
	Zhu, Dunming; Yang, Yan; Buynak, John D.; Hua, Ling; Organic and Biomolecular Chemistry; vol. 4; nb. 14; (2006); p. 2690 - 2695, View in Reaxys	
4 of 11	Effect	choleretic
	Species or Test-System	Wistar rat
	Sex	male
	Route of Application	intraduodenal
	Concentration	300 µmol/kg
	Kind of Dosing	title comp. was dissolved in dimethylsulfoxide:ethanol:water=25:15:60
	Method	bile samples were collected at 30 min after title comp. administration; biliary cholesterol concentration was determined by a modification of the ferric method; cholesterol output was analyzed
	Further Details	rats weight was 200-250 g; control: solvent, 0.5 ml
	Results	title comp. decreased biliary cholesterol conc. and did not change cholesterol output (diagram)
	Piyachaturawat, Pawinee; Chai-Ngam, Nitjagan; Chuncharunee, Aporn; Komaratat, Prayad; Suksamrarn, Api-chart; European Journal of Pharmacology; vol. 387; nb. 2; (2000); p. 221 - 227, View in Reaxys	
5 of 11	Effect	choleretic
	Species or Test-System	Wistar rat
	Sex	male
	Route of Application	intraduodenal
	Concentration	300 µmol/kg
	Kind of Dosing	title comp. was dissolved in dimethylsulfoxide:ethanol:water=25:15:60
	Method	bile samples were collected at 30 min after title comp. administration; bile acid concentration was determined enzymatically with 3α-hydroxysteroid dehydrogenase; bile acid output was analyzed
	Further Details	rats weight was 200-250 g; control: solvent, 0.5 ml
	Results	title comp. slightly decreased the concentration of bile acid as compared to the control; the bile output was not significantly affected (diagram)
	Piyachaturawat, Pawinee; Chai-Ngam, Nitjagan; Chuncharunee, Aporn; Komaratat, Prayad; Suksamrarn, Api-chart; European Journal of Pharmacology; vol. 387; nb. 2; (2000); p. 221 - 227, View in Reaxys	
6 of 11	Effect	choleretic
	Species or Test-System	Wistar rat
	Sex	male
	Route of Application	intraduodenal
	Concentration	100 - 400 µmol/kg
	Kind of Dosing	title comp. was dissolved in dimethylsulfoxide:ethanol:water=25:15:60

	Method	bile samples were collected at 30 min after title comp. administration; bile flow was determined gravimetrically; choleric activity was calculated from the slope of the dose-response curve for bile flow
	Further Details	rats weight was 200-250 g; control: solvent, 0.5 ml; choleric activity was expressed as secreted bile volume per millimole of title comp.
	Results	title comp. induced significant increasing of bile flow rate as compared to the acetophenone parent compound (diagram)
	Piyachaturawat, Pawinee; Chai-Ngam, Nitjagan; Chuncharunee, Aporn; Komaratat, Prayad; Suksamrarn, Api-chart; European Journal of Pharmacology; vol. 387; nb. 2; (2000); p. 221 - 227, View in Reaxys	
7 of 11	Effect	enzyme; inhib. of
	Endpoint of Effect	GSH level
	Species or Test-System	SPF Wistar rat
	Sex	male
	Concentration	100 - 400 µmol/l
	Kind of Dosing	added solut. title comp. in DMSO
	Exposure Period	5 - 30 min
	Method	in vitro; in isolated liver cells; 8 mg hepatocyte protein per ml, 6 ml; added title comp.; incubated; assessed total amount of reduced and oxidized glutathione (GSH) using 5,5'-dithio-bis(2-nitrobenzoic acid), and glutathione reductase by Tietze
	Further Details	at 37 deg C; in an atmosphere of 95 percent O ₂ , 5 percent CO ₂ ; in medium supplem. with 2.1 mmol/l L-lactate, 0.3 µmol/l pyruvate, 10 µmol/l glucose, 2.5 µmol/l HEPES; parallel assays for reduced glutathione using glyoxalase method by Bergmeyer
	Results	title comp. completely depleted GSH after 5 min at conc. >=200 µmol/l; depletion GSH: 50, 93, 95 percent within 5 min at 100, 200, 300 µmol/l; molar ratios GSH:title comp. 2, 1, 0.7 at conc. 100, 200, 300 µM, respect.; reaction follows a 1:1 stoichiometry
	Summer; Klein; Lichtmanegger; Wolff; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys	
8 of 11	Effect	enzyme; inhib. of
	Endpoint of Effect	GSH level
	Species or Test-System	SPF Wistar rat
	Sex	male
	Concentration	100 - 300 µmol/l
	Kind of Dosing	added solut. title comp. in DMSO
	Exposure Period	5 - 150 min
	Method	in vitro; in isolated liver cells; 8 mg hepatocyte protein per ml, 6 ml; added title comp.; incubated; assessed total amount of reduced and oxidized glutathione (GSH) using 5,5'-dithio-bis(2-nitrobenzoic acid, and glutathione reductase by Tietze
	Further Details	at 37 deg C; in an atmosphere of 95 percent O ₂ , 5 percent CO ₂ ; in medium supplem. with 2.1 mmol/l L-lactate, 0.3 µmol/l pyruvate, 10 µmol/l glucose, 2.5 µmol/l HEPES; parallel assays for reduced glutathione using glyoxalase method by Bergmeyer
	Results	after initial decrease GSH value recovered at rate ca. 4nmol/mg protein/h at conc. title comp. 100, 200 µmol/l; GSH depletion persisted during 150 min at conc. title comp. 300 µmol/l
	Summer; Klein; Lichtmanegger; Wolff; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys	
9 of 11	Effect	enzyme; examination of
	Endpoint of Effect	GSH level
	Species or Test-System	SPF Wistar rat
	Sex	male
	Concentration	100 - 300 µmol/l
	Kind of Dosing	added solut. title comp. in DMSO

	Exposure Period	5 - 150 min
	Method	in vitro; in isolated liver cells; 8 mg hepatocyte protein/ml, 6 ml; added title comp.; incubated; assessed release lactate dehydrogenase (LDH) by Summer, lipid peroxidation as thiobarbituric acid reactive materials (TBARS) and urea formation by Sies
	Further Details	at 37 deg C; in an atmosphere of 95 percent O2, 5 percent CO2; in medium supplem. with 2.1 mmol/l L-lactate, 0.3 µmol/l pyruvate, 10 µmol/l glucose, 2.5 µmol/l HEPES
	Results	title comp. slightly increased LDH release by 10 and 15 percent at 100 and 200 µM, respect.; title comp. signif. increased by 75 percent LDH release at 300 µmol/l; no lipid peroxidation at conc. <200 µM; title comp. not inhibited the formation urea from ammonia
	Summer; Klein; Lichtmanegger; Wolff ; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys	
10 of 11	Effect	enzyme; inhib. of
	Endpoint of Effect	GSH level
	Species or Test-System	SPF Wistar rat
	Sex	male
	Concentration	100 - 300 µmol/l
	Kind of Dosing	added solut. title comp. in DMSO
	Exposure Period	5 - 150 min
	Method	in vitro; in isolated liver cells; 8 mg hepatocyte protein/ml, 6 ml; added title comp.; incubated; assessed activities of microsomal ethylmorphine demethylase, aldrin epoxidase, benzo(a)pyrene hydroxylase by Wolff
	Further Details	at 37 deg C; in an atmosphere of 95 percent O2, 5 percent CO2; in medium supplem. with 2.1 mmol/l L-lactate, 0.3 µmol/l pyruvate, 10 µmol/l glucose, 2.5 µmol/l HEPES
	Results	title comp. slightly inhibited microsomal cytochrome P450 enzymes; activities ethylmorphine demethylase, aldrin epoxidase, benzo(a)pyrene hydroxylase were 85, 96 and 70 percent at 500 µM, respect.
	Summer; Klein; Lichtmanegger; Wolff ; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys	
11 of 11	Comment	compound has been tested for "in vitro" antimicrobial activity against 12 gram-positive, 8 gram-negative bacteria and against Mycobacterium smegmatis
	Rival; Grassy; Michel ; Chemical and Pharmaceutical Bulletin; vol. 40; nb. 5; (1992); p. 1170 - 1176, View in Reaxys	
Use (1)		
	Laboratory Use and Handling	References
	laboratory chemicals; in vitro studies on cellular metabolism; depleted GSH level without influence cytochrome P450 dependent enzymes, cellular ATP levels; not affected cell viability	Summer; Klein; Lichtmanegger; Wolff ; Archives of Toxicology; vol. 71; nb. 1-2; (1996); p. 127 - 129, View in Reaxys