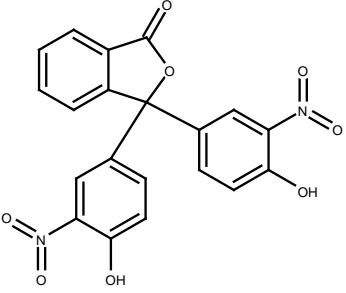
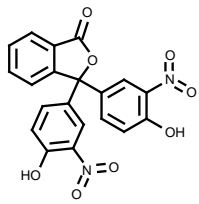


Query

Query	Results	Date
<p>1. Query</p>  <p>Search as: As drawn</p>	<p>1 substances</p>	<p>2012-01-10 05h:53m:11s (EST)</p>

Reaxys ID 368832 View in Reaxys		1/1
		<p>Chemical Name: 3,3-bis-(4-hydroxy-3-nitro-phenyl)-phthalide; 3,3-Bis-(4-hydroxy-3-nitro-phenyl)-phthalid; 3,3-bis-(4-hydroxy-3-nitrophenyl)-1-(3H)-isobenzofuranone</p> <p>Molecular Formula: C₂₀H₁₂N₂O₈</p> <p>CAS Registry Number: 33964-04-4</p> <p>Molecular Weight: 408.324</p> <p>Linear Structure Formula: C₂₀H₁₂N₂O₈</p> <p>Type of Substance: heterocyclic</p> <p>InChIKey: ILNAKHGFKXCKJG-UHFFFAOYSA-N</p> <p>Note:</p>
Patent-Specific Data (1)		
References		
Patent; Sabnis, Ram W.; Kehoe, Timothy D.; Balchunis, Robert James; US2006/222601; (2006); (A1) English, View in Reaxys		
Melting Point (5)		
Melting Point [°C]	References	
198 - 199	Mehta; Krishnamurthy; Journal of the Indian Chemical Society; vol. 40; (1963); p. 486, View in Reaxys ; Mehta et al.; Current Science; vol. 30; (1961); p. 460, View in Reaxys	
196	Hall; Chem. News J. Ind. Sci.; vol. 67; (1893); p. 93, View in Reaxys ; Patent; Clayton Aniline Co.; DE52211; Fortschr. Teerfarbenfabr. Verw. Industriezweige; vol. 2; p. 90, View in Reaxys ; Greenbaum; American Journal of Pharmacy and the Sciences Supporting Public Health (1937-1978); vol. 100; p. 378; Chem. Zentralbl.; vol. 99; nb. II; (1928); p. 984, View in Reaxys	
200 - 201	Thiel; Diehl; Sitzungsberichte der Gesellschaft zur Befoerderung der Gesamten Naturwissenschaften zu Marburg; vol. 62; p. 540; Chem. Zentralbl.; vol. 98; nb. II; (1927); p. 2669, View in Reaxys	
195	Gattermann; Chemische Berichte; vol. 32; (1899); p. 1137,1139; Chem. Zentralbl.; vol. 69; nb. II; (1898); p. 196, View in Reaxys	
197	Errera; Berte; Gazzetta Chimica Italiana; vol. 26 I; (1896); p. 265, View in Reaxys	
Crystal Phase (1)		
Description	Comment	References
Crystal structure determination	a=27.63 Angstroem, b=8.12 Angstroem, c=15.74 Angstroem, n=8.; Temperature: 296 K. Method of determination: Single Crystal X-ray Diffraction	Fitzgerald, Lawrence J.; Gerkin, Roger E.; Acta Crystallographica, Section C: Crystal Structure Communications; vol. 54; nb. 4; (1998); p. 535 - 539, View in Reaxys
Crystal Property Description (1)		
Colour & Other Properties	References	
light-yellow	Patent; Sabnis, Ram W.; Kehoe, Timothy D.; Balchunis, Robert James; US2006/222601; (2006); (A1) English, View in Reaxys	
Crystal System (1)		
Crystal System	References	
rhombic	Fitzgerald, Lawrence J.; Gerkin, Roger E.; Acta Crystallographica, Section C: Crystal Structure Communications; vol. 54; nb. 4; (1998); p. 535 - 539, View in Reaxys	
Density of the Crystal (1)		
Density of the Crystal [gcm-3]	References	
1.535	Fitzgerald, Lawrence J.; Gerkin, Roger E.; Acta Crystallographica, Section C: Crystal Structure Communications; vol. 54; nb. 4; (1998); p. 535 - 539, View in Reaxys	
Solution Behaviour (MCS) (1)		
1 of 1	Description	Dissolving capacity
	Iwachido,T.; Bulletin of the Chemical Society of Japan; vol. 44; (1971); p. 1835 - 1840, View in Reaxys	
Space Group (1)		

Space Group	References	
60	Fitzgerald, Lawrence J.; Gerkin, Roger E. ; Acta Crystallographica, Section C: Crystal Structure Communications; vol. 54; nb. 4; (1998); p. 535 - 539, View in Reaxys	
NMR Spectroscopy (1)		
1 of 1	Nucleus	¹ H
	Solvents	dimethylsulfoxide-d6
	Original Text	¹ H-NMR (DMSO-d ₆): δ 9.67 (s, 2H, 2OH), 6.71-7.16 (m, 6H, aromatic), 7.46-7.98 (m, 4H, aromatic) ppm
	Comment	Signals given
	Patent; Sabnis, Ram W.; Kehoe, Timothy D.; Balchunis, Robert James ; US2006/222601; (2006); (A1) English, View in Reaxys	
IR Spectroscopy (1)		
Description	Original Text	References
in KBr	IR (KBr): 3262, 1766, 1627, 1538, 1423 cm ⁻¹	Patent; Sabnis, Ram W.; Kehoe, Timothy D.; Balchunis, Robert James ; US2006/222601; (2006); (A1) English, View in Reaxys
Mass Spectrometry (1)		
Comment	References	
Molecular peak	Patent; Sabnis, Ram W.; Kehoe, Timothy D.; Balchunis, Robert James ; US2006/222601; (2006); (A1) English, View in Reaxys	
UV/VIS Spectroscopy (1)		
Description	Comment	References
Spectrum	bei pH 8 und 14 im sichtbaren Gebiet.	Thiel; Diehl ; Sitzungsberichte der Gesellschaft zur Befoerderung der Gesamten Naturwissenschaften zu Marburg; vol. 62; p. 489,498, View in Reaxys