Query

	Query	Results	Date
1. Query	 Search as: Substructure: on all atoms	13 substances in Reaxys	2015-06-07 05h:52m:59s (EST)
2. Query	(1. Query) AND itemno in (1,2,4,7,13)	5 substances in Reaxys	2015-06-07 05h:56m:03s (EST)
3. Query	(2. Query) AND NOT itemno in (3,4,5)	2 substances in Reaxys	2015-06-07 05h:56m:25s (EST)

CAS Registry Number: 7616-35-5
Chemical Name: hexaazabenzene; cyclo-N6
Linear Structure Formula: N_6
Molecular Formula: N_6
Molecular Weight: 84.0402
InChI Key: YRBKSJIXFZPPGF-UHFFFAOYSA-N
Note:

Druglikeness (1)

1 of 1	LogP	-2.958
	H Bond Donors	0
	H Bond Acceptors	6
	Rotatable Bonds	0
	TPSA	77.34
	Lipinski Number	4
	Veber Number	2

Dissociation Energy (1)

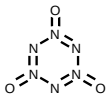
Comment (Dissociation Energy)	References
information on dissociation energy	**Ionov, S. P.; Orlovskii, V. P.; Kirilenko, V. V.**; Doklady Physical Chemistry (Translation of the physical chemistry section of Doklady Akademii Nauk); **vol.** 327; (1992); p. 596 - 598; Doklady Akademii Nauk SSSR; **vol.** 327; (1992); p. 521 - 523 ; (from Gmelin), View in Reaxys

Quantum Chemical Calculations (30)

Calculated Properties	Method (Quantum Chemical Calculations)	References
Molecular orbitals	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Noyman, Moran; Zilberg, Shmuel; Haas, Yehuda**; Journal of Physical Chemistry A; **vol.** 113; nb. 26; (2009); p. 7376 - 7382 ; (from Gmelin), View in Reaxys
Atom distances, angles; Contour map; Molecular orbitals; Electronic energy levels; Total energy	Electron correlation and CI calcn.	**Hill, J. Grant; Cooper, David L.; Karadakov, Peter B.**; Journal of Physical Chemistry A; **vol.** 110; nb. 25; (2006); p. 7913 - 7917 ; (from Gmelin), View in Reaxys
Atom distances, angles; NMR shifts, signals, intensities, transition moments	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Duan, Hongxia; Gong, Zhen; Cheng, Jiagao; Zhu, Weiliang; Chen, Kaixian; Jiang, Hualiang**; Journal of Physical Chemistry A; **vol.** 110; nb. 44; (2006); p. 12236 - 12240 ; (from Gmelin), View in Reaxys
NMR shifts, signals, intensities, transition moments	Electron correlation and CI calcn.	**Duan, Hongxia; Gong, Zhen; Cheng, Jiagao; Zhu, Weiliang; Chen, Kaixian; Jiang, Hualiang**; Journal of Physical Chemistry A; **vol.** 110; nb. 44; (2006); p. 12236 - 12240 ; (from Gmelin), View in Reaxys
Atom distances, angles	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Inagaki, Satoshi; Goto, Naomi**; Journal of the American Chemical Society; **vol.** 109; nb. 11; (1987); p. 3234 - 3240, View in Reaxys; **Jungnickel, Gerd; Frauenheim, Thomas; Jackson, Koblar Alan**; Journal of Chemical Physics; **vol.** 112; nb. 3; (2000); p. 1295 - 1305, View in Reaxys; **Ohanessian, G.; Hiberty, P. C.; Lefour, J.-M.; Flament, J.-P.; Shaik, S. S.**; Inorganic Chemistry; **vol.** 27; (1988); p. 2219 - 2224, View in Reaxys; **Glukhovtsev, Mikhail N.; Jiao, Haijun; Von Schleyer, Paul Rague**; Inorganic Chemistry; **vol.** 35; nb. 24; (1996); p. 7124 - 7133, View in Reaxys; **Duan, Hong-Xia; Li, Qian-Shu**; Chemical Physics Letters; **vol.** 432; nb. 1-3; (2006); p. 331 - 335 ; (from Gmelin), View in Reaxys
Atom distances, angles; Total energy	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-al-	**Engelberts, Jeroen J.; Havenith, Remco W. A.; Van Lenthe, Joop H.; Jenneskens, Leonardus W.; Fowler, Patrick W.**; Inorganic Chemistry; **vol.** 44; nb. 15; (2005); p. 5266 - 5272 ; (from Gmelin), View in Reaxys

	pha, Hartree-Fock)	
Contour map; Total energy; Shielding constant	Valence bond calcns.	**Engelberts, Jeroen J.; Havenith, Remco W. A.; Van Lenthe, Joop H.; Jenneskens, Leonardus W.; Fowler, Patrick W.**; Inorganic Chemistry; **vol.** 44; nb. 15; (2005); p. 5266 - 5272 ; (from Gmelin), View in Reaxys
Atom distances, angles; Dissociation energy, bonding energy	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Radhika Devi; Shrivastava, Keshav N.**; Chemical Physics Letters; **vol.** 396; nb. 4-6; (2004); p. 238 - 244, View in Reaxys; **Glukhovtsev, Mikhail N.; Jiao, Haijun; Von Schleyer, Paul Rague**; Inorganic Chemistry; **vol.** 35; nb. 24; (1996); p. 7124 - 7133 ; (from Gmelin), View in Reaxys
Atom distances, angles; Vibrational constants	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Lauderdale, Walter J.; Stanton, John F.; Bartlett, Rodney J.**; Journal of Physical Chemistry; **vol.** 96; nb. 3; (1992); p. 1173 - 1178, View in Reaxys; **Straka, Michal**; Chemical Physics Letters; **vol.** 358; nb. 5-6; (2002); p. 531 - 536 ; (from Gmelin), View in Reaxys
Atom distances, angles; Equilibrium internuclear distance	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Li, Qian Shu; Liu, Yong Dong**; Journal of Physical Chemistry A; **vol.** 106; nb. 41; (2002); p. 9538 - 9542 ; (from Gmelin), View in Reaxys
Atom distances, angles; Equilibrium internuclear distance	Electron correlation and CI calcn.	**Li, Qian Shu; Liu, Yong Dong**; Journal of Physical Chemistry A; **vol.** 106; nb. 41; (2002); p. 9538 - 9542 ; (from Gmelin), View in Reaxys
Atom distances, angles; Vibrational constants; IR bands, intensities, transition moments; Raman bands, intensities, transition moments	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Tobita, Motoi; Bartlett, Rodney J.**; Journal of Physical Chemistry A; **vol.** 105; nb. 16; (2001); p. 4107 - 4113 ; (from Gmelin), View in Reaxys
Atom distances, angles; Vibrational constants; IR bands, intensities, transition moments; Raman bands, intensities, transition moments	further quantum chemical calcns.	**Tobita, Motoi; Bartlett, Rodney J.**; Journal of Physical Chemistry A; **vol.** 105; nb. 16; (2001); p. 4107 - 4113 ; (from Gmelin), View in Reaxys
NMR shifts, signals, intensities, transition moments	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Ragué Schleyer, Paul von; Jiao, Haijuan; van Eikema Hommes, Nicolaas J. R.; Malkin, Vladimir G.; Malkina, Olga L.**; Journal of the American Chemical Society; **vol.** 119; (1997); p. 12669 - 12670 ; (from Gmelin), View in Reaxys
Total energy	Electron correlation and CI calcn.	**Saxe, Paul; Schaefer, Henry F.**; Journal of the American Chemical Society; **vol.** 105; nb. 7; (1983); p. 1760 - 1764, View in Reaxys; **Glukhovtsev, Mikhail N.; Dransfeld, Alk; Schleyer, Paul von R.**; Journal of Physical Chemistry; **vol.** 100; nb. 32; (1996); p. 13447 - 13454, View in Reaxys; **Glukhovtsev, Mikhail N.; Schleyer, Paul von Ragué**; Chemical Physics Letters; **vol.** 198; (1992); p. 547 - 554 ; (from Gmelin), View in Reaxys
Excited states; Total energy	Electron correlation and CI calcn.	**Hiberty, P. C.; Ohanessian, G.; Shaik, S. S.; Flament, J. P.**; Pure and Applied Chemistry; **vol.** 65; (1993); p. 35 - 46 ; (from Gmelin), View in Reaxys
Atom distances, angles	Electron correlation and CI calcn.	**Glukhovtsev, M. N.; Schleyer, P. von R.**; Chemical Physics Letters; **vol.** 204; (1993); p. 394 - 394 ; (from Gmelin), View in Reaxys
Atom distances, angles; Population analysis, charge distribution	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Li, Jun; Liu, Chun-Wan; Lu, Jia-Xi**; Journal of Molecular Structure; **vol.** 280; (1993); p. 223 - 232 ; (from Gmelin), View in Reaxys

Total energy; Atom distances, angles; Molecular orbitals	Electron correlation and CI calcn.	**Glukhovtsev, Mikhail N.; Schleyer, Paul von Rague**; Chemical Physics Letters; **vol.** 198; (1992); p. 547 - 554 ; (from Gmelin), View in Reaxys
Atom distances, angles; Oscillator strength, transition probability; Total energy; Vibrational constants; IR bands, intensities, transition moments	Electron correlation and CI calcn.	**Ha, Tae-Kyu; Nguyen, Minh Tho**; Chemical Physics Letters; **vol.** 195; (1992); p. 179 - 183 ; (from Gmelin), View in Reaxys
Total energy	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Glukhovtsev, Mikhail N.; Schleyer, Paul von Rague**; Chemical Physics Letters; **vol.** 198; (1992); p. 547 - 554, View in Reaxys; **Nagase, Shigeru; Ito, Keiji**; Chemical Physics Letters; **vol.** 126; (1986); p. 43 - 47 ; (from Gmelin), View in Reaxys
Atom distances, angles; Vibrational constants	Electron correlation and CI calcn.	**Lauderdale, Walter J.; Stanton, John F.; Bartlett, Rodney J.**; Journal of Physical Chemistry; **vol.** 96; nb. 3; (1992); p. 1173 - 1178 ; (from Gmelin), View in Reaxys
Atom distances, angles; Total energy	Electron correlation and CI calcn.	**Engelke, Ray**; Journal of Physical Chemistry; **vol.** 96; nb. 26; (1992); p. 10789 - 10792 ; (from Gmelin), View in Reaxys
Equilibrium internuclear distance; IR bands, intensities, transition moments; Total energy; Rotational constants; Dissociation energy, bonding energy	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Engelke, Ray**; Journal of Physical Chemistry; **vol.** 93; (1989); p. 5722 - 5727 ; (from Gmelin), View in Reaxys
NMR shifts, signals, intensities, transition moments; Vibrational constants	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Engelke, Ray**; Journal of Physical Chemistry; **vol.** 93; (1989); p. 5722 - 5727 ; (from Gmelin), View in Reaxys
Population analysis, charge distribution	Electron correlation and CI calcn.	**Inagaki, Satoshi; Goto, Naomi**; Journal of the American Chemical Society; **vol.** 109; nb. 11; (1987); p. 3234 - 3240 ; (from Gmelin), View in Reaxys
Correlation energy	Semi-empirical NDO calcns. (CNDO, INDO, MINDO, PCILO)	**Oles, Andrzej M.; Fulde, Peter; Boehm, Michael C.**; Chemical Physics; **vol.** 117; (1987); p. 385 - 404 ; (from Gmelin), View in Reaxys
Total energy; Equilibrium internuclear distance; Atom distances, angles; Vibrational constants	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Saxe, Paul; Schaefer, Henry F.**; Journal of the American Chemical Society; **vol.** 105; nb. 7; (1983); p. 1760 - 1764 ; (from Gmelin), View in Reaxys
Atom distances, angles; Transition energies	Electron correlation and CI calcn.	**Ha, Tae-Kyu; Cimiraglia, R.; Nguyen, Minh Tho**; Chemical Physics Letters; **vol.** 83; (1981); p. 317 - 319 ; (from Gmelin), View in Reaxys
Atom distances, angles; Transition energies; Wave function	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Ha, Tae-Kyu; Cimiraglia, R.; Nguyen, Minh Tho**; Chemical Physics Letters; **vol.** 83; (1981); p. 317 - 319 ; (from Gmelin), View in Reaxys



CAS Registry Number: 123119-80-2
Chemical Name: 1,3,5-trioxo-cyclo-N6
Linear Structure Formula: N_6O_3
Molecular Formula: N_6O_3
Molecular Weight: 132.038
InChI Key: QYNMABHLRRNRDG-UHFFFAOYSA-N
Note:

Druglikeness (1)

1 of 1	LogP	-0.033
	H Bond Donors	0
	H Bond Acceptors	3
	Rotatable Bonds	0
	TPSA	115.05
	Lipinski Number	4
	Veber Number	2

Quantum Chemical Calculations (7)

Calculated Properties	Method (Quantum Chemical Calculations)	References
Atom distances, angles; Dissociation energy, bonding energy	further quantum chemical calcns.	**Noyman, Moran; Zilberg, Shmuel; Haas, Yehuda**; Journal of Physical Chemistry A; **vol.** 113; nb. 26; (2009); p. 7376 - 7382 ; (from Gmelin), View in Reaxys
Dissociation energy, bonding energy	Electron correlation and CI calcn.	**Noyman, Moran; Zilberg, Shmuel; Haas, Yehuda**; Journal of Physical Chemistry A; **vol.** 113; nb. 26; (2009); p. 7376 - 7382 ; (from Gmelin), View in Reaxys
Dissociation energy, bonding energy; Molecular orbitals	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Noyman, Moran; Zilberg, Shmuel; Haas, Yehuda**; Journal of Physical Chemistry A; **vol.** 113; nb. 26; (2009); p. 7376 - 7382 ; (from Gmelin), View in Reaxys
Total energy; Atom distances, angles; Vibrational constants; IR bands, intensities, transition moments; Population analysis, charge distribution	Ab initio calcns. (LCAO, GO SCF, DIM, SAMO, X-alpha, Hartree-Fock)	**Wilson, Kenneth J.; Perera, S. Ajith; Bartlett, Rodney J.; Watts, John D.**; Journal of Physical Chemistry A; **vol.** 105; nb. 32; (2001); p. 7693 - 7699 ; (from Gmelin), View in Reaxys
Total energy; Atom distances, angles; Vibrational constants; Population analysis, charge distribution	Electron correlation and CI calcn.	**Wilson, Kenneth J.; Perera, S. Ajith; Bartlett, Rodney J.; Watts, John D.**; Journal of Physical Chemistry A; **vol.** 105; nb. 32; (2001); p. 7693 - 7699 ; (from Gmelin), View in Reaxys
Total energy; Atom distances, angles; Vibrational constants; IR bands, intensities, transition moments	further quantum chemical calcns.	**Wilson, Kenneth J.; Perera, S. Ajith; Bartlett, Rodney J.; Watts, John D.**; Journal of Physical Chemistry A; **vol.** 105; nb. 32; (2001); p. 7693 - 7699 ; (from Gmelin), View in Reaxys
Atom distances, angles	Semi-empirical NDO calcns. (CNDO, INDO, MINDO, PCILO)	**Stankevich, I. V.; Chistyakov, A. L.; Shur, V. B.; Vol'pin, M. E.**; Doklady Chemistry (English Translation); **vol.** 313; (1990); p. 194 - 195; Doklady Akademii Nauk SSSR; **vol.** 313; (1990); p. 118 - 120 ; (from Gmelin), View in Reaxys