4-NITROBENZOFUROXAN

Other names:	4-Nitrobenzofuroxan
	B2789
	Nitrobenzofuroxan
	2,1,3-Benzoxadiazole, 4-nitro-, 1-oxide
	4-Nitrobenzofuroxan-1-oxide
Inchi:	InChI=1S/C6H3N3O4/c10-8(11)4-2-1-3-5-6(4)7-13-9(5)12/h1-3H
InchiKey:	XUCKCDGEIRMZPM-UHFFFAOYSA-N
Formula:	C6H3N3O4
SMILES:	O=[N+]([O-])c1cccc2c1no[n+]2[O-]
Mol. weight [g/mol]:	181.11

Physical Properties

Property code	Value	Unit	Source
hf	294.47	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-2.57		Cheméo Relay (1.0)
logp	0.369		Crippen Method
mcvol	105.600	ml/mol	McGowan Method
tf	395.91	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18771852&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point