

Benzofurazan, 4,6-dinitro-, 1-oxide

Other names:	2,1,3-Benzoxadiazole, 4,6-dinitro-, 1-oxide 4,6-Dinitrobenzofurazan 1-oxide 4,6-Dinitrobenzofurazan oxide 4,6-Dinitrobenzofuroxan
Inchi:	InChI=1S/C6H2N4O6/c11-8(12)3-1-4(9(13)14)6-5(2-3)10(15)16-7-6/h1-2H
InchiKey:	YHBBUAULQKLKMW-UHFFFAOYSA-N
Formula:	C6H2N4O6
SMILES:	O=[N+](O)c1cc([N+](=O)[O-])c2no[n+](O)c2c1
Mol. weight [g/mol]:	226.10
CAS:	5128-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.61		Crippen Method
logp	0.278		Crippen Method
mcpvol	123.020	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.73	kJ/mol	452.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5128289&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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