

Benzofuroxan

Other names:	Benzofurazan, 1-oxide Benzofuroxane Benzofurazan oxide Benzofurazan N-oxide Benzo[1,2,5]oxadiazole 3-oxide 2,1,3-Benzoxadiazole 1-oxide NSC 19930 1-benzo-2-oxa-1,3-diazole oxide
Inchi:	InChI=1S/C6H4N2O2/c9-8-6-4-2-1-3-5(6)7-10-8/h1-4H
InchiKey:	OKEAMBAZBICIFP-UHFFFAOYSA-N
Formula:	C6H4N2O2
SMILES:	[O-][n+]1onc2cccc21
Mol. weight [g/mol]:	136.11
CAS:	480-96-6

Physical Properties

Property code	Value	Unit	Source
chs	-3151.60 ± 1.20	kJ/mol	NIST Webbook
hf	298.50 ± 2.20	kJ/mol	NIST Webbook
hfs	218.90 ± 1.40	kJ/mol	NIST Webbook
hsub	79.60 ± 1.70	kJ/mol	NIST Webbook
hsub	79.60 ± 1.70	kJ/mol	NIST Webbook
log10ws	-8.30		Crippen Method
logp	0.461		Crippen Method
mcvol	88.180	ml/mol	McGowan Method

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=C480966&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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