5-Methoxybenzofurazan, 1-oxide

Other names: 5-Methoxy-2,1,3-benzoxadiazole 1-oxide
Benzofurazan, 5-methoxy-, 1-oxide
5-Methoxybenzofuran-1-oxide
Inchi: InChI=1S/C7H6N2O3/c1-11-5-2-3-7-6(4-5)8-12-9(7)10/h2-4H,1H3
InchiKey: ABSKHUSUHODMEL-UHFFFAOYSA-N
Formula: C7H6N2O3
SMILES: COc1ccc2c(c1)no[n+]2[O-]
Mol. weight [g/mol]: 166.13
CAS: 7791-49-3

Physical Properties

Property code	Value	Unit	Source
chs	-3664.40 ± 3.20	kJ/mol	NIST Webbook
hf	148.30 ± 3.70	kJ/mol	NIST Webbook
hfs	52.30 ± 3.30	kJ/mol	NIST Webbook
hsub	96.00 ± 1.60	kJ/mol	NIST Webbook
hsub	96.00 ± 1.60	kJ/mol	NIST Webbook
log10ws	-8.42		Crippen Method
logp	0.470		Crippen Method
mcvol	108.140	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7791493&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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