Benzofurazan, 5-methyl-, 1-oxide

Other names:	5-Methylbenzofurazan oxide
	5-Methylbenzofurazan N-oxide
	5-Methylbenzofurazan 1-oxide
	5-Methylbenzofuroxan
Inchi:	InChI=1S/C7H6N2O2/c1-5-2-3-7-6(4-5)8-11-9(7)10/h2-4H,1H3
InchiKey:	HCWVKDOCXDWFEH-UHFFFAOYSA-N
Formula:	C7H6N2O2
SMILES:	Cc1ccc2c(c1)no[n+]2[O-]
Mol. weight [g/mol]:	150.13
CAS:	19164-41-1

Physical Properties

Property code	Value	Unit	Source
chs	-3787.30 ± 1.50	kJ/mol	NIST Webbook
hf	267.40 ± 2.20	kJ/mol	NIST Webbook
hfs	175.20 ± 1.80	kJ/mol	NIST Webbook
hsub	92.20 ± 1.20	kJ/mol	NIST Webbook
hsub	92.20 ± 1.20	kJ/mol	NIST Webbook
log10ws	-8.78		Crippen Method
logp	0.770		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19164411&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

Latest version available from:

https://www.chemeo.com/cid/28-459-2/Benzofurazan-5-methyl-1-oxide.pdf

Generated by Cheméo on 2024-10-12 06:58:28.188512554 +0000 UTC m=+3297170.825481806.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.