

Morpholine, 4-methyl-, 4-oxide

Other names:	4-Methylmorpholine 4-oxide N-Methylmorpholine N-oxide N-Methylmorpholine 4-oxide N-Methylmorpholine oxide 4-methylmorpholine 4-oxide monohydrate
Inchi:	InChI=1S/C5H11NO2/c1-6(7)2-4-8-5-3-6/h2-5H2,1H3
InchiKey:	LFTLOKWAGJYHHR-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	C[N+](O)CCOCC1
Mol. weight [g/mol]:	117.15
CAS:	7529-22-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.52		Crippen Method
logp	-0.039		Crippen Method
mcvol	92.170	ml/mol	McGowan Method
tf	457.40 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.80	kJ/mol	457.40	NIST Webbook
hfust	18.80	kJ/mol	457.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7529228&Units=SI
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

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
tf:	Normal melting (fusion) point

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