

N-MORPHOLINOMETHYL-ISOPROPYL-SULFIDE

Other names:	1-Isopropylthiomethylmorpholine
Inchi:	InChI=1S/C8H17NOS/c1-8(2)11-7-9-3-5-10-6-4-9/h8H,3-7H2,1-2H3
InchiKey:	YXTBTNKSywaUtA-UHFFFAOYSA-N
Formula:	C8H17NOS
SMILES:	CC(C)SCN1CCOCC1
Mol. weight [g/mol]:	175.30

Physical Properties

Property code	Value	Unit	Source
hvap	61.22	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
logp	1.418		Crippen Method
mcvol	144.920	ml/mol	McGowan Method
tb	508.92	K	Cheméo Relay (1.0)
tf	250.42	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77422345&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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