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