1-BUTANETHIOL, 4-(METHYLTHIO)-

Other names: 5-Thia-1-hexanethiol
Inchi: InChI=1S/C5H12S2/c1-7-5-3-2-4-6/h6H,2-5H2,1H3
InchiKey: VLSYQLPMYBNHCJ-UHFFFAOYSA-N
Formula: C5H12S2
SMILES: CSCCCCS
Mol. weight [g/mol]: 136.29

Physical Properties

Property code	Value	Unit	Source
hf	-93.02	kJ/mol	Cheméo Relay (1.0)
hfus	16.88	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Cheméo Relay (1.0)
logp	2.059		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1151.00		NIST Webbook
tb	475.13	K	Cheméo Relay (1.0)
tc	699.61	K	Cheméo Relay (1.0)
tf	221.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.39	J/mol×K	445.44	Joback Method
cpg	223.30	J/mol×K	481.34	Joback Method
cpg	233.71	J/mol×K	517.23	Joback Method
cpg	243.64	J/mol×K	553.13	Joback Method
cpg	253.08	J/mol×K	589.03	Joback Method
cpg	262.05	J/mol×K	624.92	Joback Method
cpg	270.56	J/mol×K	660.82	Joback Method

Sources

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=C66890946&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point