

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]:	136.28
CAS:	66890-94-6

Physical Properties

Property code	Value	Unit	Source
gf	53.73	kJ/mol	Joback Method
hf	-66.18	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.28	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.059		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1151.00		NIST Webbook
tb	445.44	K	Joback Method
tc	660.82	K	Joback Method
tf	216.97	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66890946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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