

3-Mercapto-3-methylbutanol

Other names:	3-Methyl-3-sulfanyl-1-butanol 3-Mercapto-3-methyl-1-butanol 3-Mercapto-3-methyl-butan-1-ol 3-Methyl-3-sulfanylbutan-1-ol 3-Methyl-3-sulfanylbutanol-1-ol
Inchi:	InChI=1S/C5H12OS/c1-5(2,7)3-4-6/h6-7H,3-4H2,1-2H3
InchiKey:	GBCGIJAYTBMFHI-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CC(C)(S)CCO
Mol. weight [g/mol]:	120.21
CAS:	34300-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-113.37	kJ/mol	Joback Method
hf	-269.03	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.077		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	938.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1677.00		NIST Webbook
tb	465.61	K	Joback Method
tc	659.33	K	Joback Method
tf	245.81	K	Joback Method
vc	0.378	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.31	J/molxK	465.61	Joback Method
cpg	225.15	J/molxK	497.90	Joback Method
cpg	234.43	J/molxK	530.18	Joback Method
cpg	243.17	J/molxK	562.47	Joback Method
cpg	251.41	J/molxK	594.76	Joback Method
cpg	259.16	J/molxK	627.05	Joback Method
cpg	266.46	J/molxK	659.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34300942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvap:	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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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