

3-Mercapto-2-methylpentanol

Other names:	2-methyl-3-sulfanyl-pentan-1-ol 1-Pentanol, 3-mercapto-2-methyl-
Inchi:	InChI=1S/C6H14OS/c1-3-6(8)5(2)4-7/h5-8H,3-4H2,1-2H3
InchiKey:	HABNNYNSJFKZFE-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CCC(S)C(C)CO
Mol. weight [g/mol]:	134.24

Physical Properties

Property code	Value	Unit	Source
gf	-112.67	kJ/mol	Joback Method
hf	-291.48	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.323		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1084.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	490.84	K	Joback Method
tc	679.02	K	Joback Method
tf	224.66	K	Joback Method
vc	0.432	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.45	J/mol×K	490.84	Joback Method
cpg	264.05	J/mol×K	522.20	Joback Method
cpg	274.16	J/mol×K	553.57	Joback Method
cpg	283.81	J/mol×K	584.93	Joback Method
cpg	293.00	J/mol×K	616.29	Joback Method
cpg	301.75	J/mol×K	647.66	Joback Method
cpg	310.08	J/mol×K	679.02	Joback Method

Sources

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=C227456271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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