

4-Mercapto-3-methylpentan-2-ol

Inchi: InChI=1S/C6H14OS/c1-4(5(2)7)6(3)8/h4-8H,1-3H3
InchiKey: IAEUQPZVOWVIES-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CC(O)C(C)C(C)S
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
gf	-115.11	kJ/mol	Joback Method
hf	-296.76	kJ/mol	Joback Method
hfus	8.86	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.322		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
ripol	1063.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1022.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
tb	490.40	K	Joback Method
tc	682.69	K	Joback Method
tf	209.66	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.69	J/mol×K	490.40	Joback Method
cpg	264.59	J/mol×K	522.45	Joback Method
cpg	274.99	J/mol×K	554.50	Joback Method
cpg	284.88	J/mol×K	586.54	Joback Method
cpg	294.29	J/mol×K	618.59	Joback Method
cpg	303.24	J/mol×K	650.64	Joback Method
cpg	311.73	J/mol×K	682.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R282456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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