3-Pentanethiol, 3-methyl-

Other names: 3-Methyl-3-pentanethiol
3-methylpentane-3-thiol
Inchi: InChI=1S/C6H14S/c1-4-6(3,7)5-2/h7H,4-5H2,1-3H3
InchiKey: AJWVDGABWLKIGT-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCC(C)(S)CC
Mol. weight [g/mol]: 118.24
CAS: 1639-03-8

Physical Properties

Property code	Value	Unit	Source
gf	31.87	kJ/mol	Joback Method
hf	-137.44	kJ/mol	Joback Method
hfus	7.92	kJ/mol	Joback Method
hvap	34.39	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.495		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
tb	396.31	K	Joback Method
tc	598.05	K	Joback Method
tf	196.26	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.50	J/mol×K	396.31	Joback Method
cpg	219.51	J/mol×K	429.93	Joback Method
cpg	231.80	J/mol×K	463.56	Joback Method
cpg	243.40	J/mol×K	497.18	Joback Method
cpg	254.34	J/mol×K	530.80	Joback Method

cpg	264.66	J/mol×K	564.43	Joback Method
cpg	274.38	J/mol×K	598.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1639038&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume