1-Pentanethiol, 3-methyl-

Other names: 3-Methylpentan-1-thiol
Inchi: InChI=1S/C6H14S/c1-3-6(2)4-5-7/h6-7H,3-5H2,1-2H3
InchiKey: WUACDJJGMSFOGF-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCC(C)CCS
Mol. weight [g/mol]: 118.24
CAS: 1633-88-1

Physical Properties

Property code	Value	Unit	Source
gf	26.59	kJ/mol	Joback Method
hf	-133.97	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	35.30	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.352		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	877.00		NIST Webbook
tb	399.10	K	Joback Method
tc	592.27	K	Joback Method
tf	178.84	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.79	J/mol×K	399.10	Joback Method
cpg	216.65	J/mol×K	431.30	Joback Method
cpg	228.00	J/mol×K	463.49	Joback Method
cpg	238.86	J/mol×K	495.69	Joback Method
cpg	249.24	J/mol×K	527.88	Joback Method
cpg	259.15	J/mol×K	560.08	Joback Method
cpg	268.61	J/mol×K	592.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633881&Units=SI

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