3-Pentanethiol, 2-methyl-

Inchi: InChI=1S/C6H14S/c1-4-6(7)5(2)3/h5-7H,4H2,1-3H3
InchiKey: NTRKGRUMBHBCAM-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCC(S)C(C)C
Mol. weight [g/mol]: 118.24
CAS: 1639-04-9

Physical Properties

Property code	Value	Unit	Source
gf	24.15	kJ/mol	Joback Method
hf	-139.25	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	34.91	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.351		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	408.75 ± 0.20	K	NIST Webbook
tc	596.55	K	Joback Method
tf	163.84	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.76	J/mol×K	398.66	Joback Method
cpg	217.01	J/mol×K	431.64	Joback Method
cpg	228.72	J/mol×K	464.62	Joback Method
cpg	239.90	J/mol×K	497.61	Joback Method
cpg	250.57	J/mol×K	530.59	Joback Method
cpg	260.75	J/mol×K	563.57	Joback Method
cpg	270.44	J/mol×K	596.55	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=C1639049&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume