3-sulfanyl-pentan-1-ol

Other names: 3-mercaptopentanol
Inchi: InChI=1S/C5H12OS/c1-2-5(7)3-4-6/h5-7H,2-4H2,1H3
InchiKey: PRJACVDGNSZBLE-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CCC(S)CCO
Mol. weight [g/mol]: 120.21

Physical Properties

Property code	Value	Unit	Source
gf	-118.65	kJ/mol	Joback Method
hf	-265.56	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.077		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	468.40	K	Joback Method
tc	654.54	K	Joback Method
tf	228.39	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.35	J/mol×K	468.40	Joback Method
cpg	221.54	J/mol×K	499.42	Joback Method
cpg	230.32	J/mol×K	530.45	Joback Method
cpg	238.70	J/mol×K	561.47	Joback Method

cpg	246.71	J/mol×K	592.49	Joback Method
cpg	254.35	J/mol×K	623.52	Joback Method
cpg	261.63	J/mol×K	654.54	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=R292027&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