3-hydroxy-2-thiabutane

Inchi: InChI=1S/C4H10OS/c1-3(5)4(2)6/h3-6H,1-2H3
InchiKey: MJQWABQELVFQJL-UHFFFAOYSA-N
Formula: C4H10OS
SMILES: CC(O)C(C)S
Mol. weight [g/mol]: 106.19

Physical Properties

Property code	Value	Unit	Source
gf	-129.51	kJ/mol	Joback Method
hf	-250.20	kJ/mol	Joback Method
hfus	7.20	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.685		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	941.00		NIST Webbook
tb	445.08	K	Joback Method
tc	637.41	K	Joback Method
tf	202.12	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.81	J/mol×K	445.08	Joback Method
cpg	182.01	J/mol×K	477.13	Joback Method
cpg	189.85	J/mol×K	509.19	Joback Method
cpg	197.33	J/mol×K	541.24	Joback Method
cpg	204.45	J/mol×K	573.30	Joback Method
cpg	211.24	J/mol×K	605.35	Joback Method
cpg	217.69	J/mol×K	637.41	Joback Method

Sources

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=R223848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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