L(+)-3-amino-4-mercapto-1-butanol

Inchi: InChI=1S/C4H11NOS/c5-4(3-7)1-2-6/h4,6-7H,1-3,5H2
InchiKey: AOHVPQZLNWRCTF-UHFFFAOYSA-N
Formula: C4H11NOS
SMILES: NC(CS)CCO
Mol. weight [g/mol]: 121.20

Physical Properties

Property code	Value	Unit	Source
gf	-60.62	kJ/mol	Joback Method
hf	-211.13	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	58.17	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.374		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	5243.40	kPa	Joback Method
tb	518.05	K	Joback Method
tc	717.52	K	Joback Method
tf	300.38	K	Joback Method
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.92	J/mol×K	518.05	Joback Method
cpg	228.33	J/mol×K	551.29	Joback Method
cpg	236.31	J/mol×K	584.54	Joback Method
cpg	243.89	J/mol×K	617.78	Joback Method
cpg	251.08	J/mol×K	651.03	Joback Method
cpg	257.88	J/mol×K	684.27	Joback Method
cpg	264.32	J/mol×K	717.52	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=B6004560&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