L-Cysteine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C14H25NO6S/c1-6-19-13(17)15-11(8-22-14(18)20-7-2)12(16)21-10(5)9(3)4/h9
InchiKey: PAEBNKSBIBNKLW-NFJWQWPMSA-N
Formula: C14H25NO6S
SMILES: CCOC(=O)NC(CSC(=O)OCC)C(=O)OC(C)C(C)C
Mol. weight [g/mol]: 335.42

Physical Properties

Property code	Value	Unit	Source
gf	-519.57	kJ/mol	Joback Method
hf	-987.19	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.579		Crippen Method
mcvol	256.770	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2073.90		NIST Webbook
tb	866.22	K	Joback Method
tc	1073.72	K	Joback Method
tf	506.08	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.30	J/mol×K	866.22	Joback Method
cpg	799.18	J/mol×K	900.80	Joback Method
cpg	810.83	J/mol×K	935.39	Joback Method
cpg	821.24	J/mol×K	969.97	Joback Method
cpg	830.39	J/mol×K	1004.55	Joback Method
cpg	838.26	J/mol×K	1039.14	Joback Method
cpg	844.85	J/mol×K	1073.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502062&Units=SI
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

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