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

Inchi: InChI=1S/C12H23NO4S/c1-6-16-12(15)13-10(7-18-5)11(14)17-9(4)8(2)3/h8-10H,6-7H2,1

InchiKey: JCUMFYLLNLUYLQ-YHMJZVADSA-N

Formula: C12H23NO4S

SMILES: CCOC(=O)NC(CSC)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 277.38

Physical Properties

Property code	Value	Unit	Source
gf	-302.49	kJ/mol	Joback Method
hf	-701.11	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	72.71	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.052		Crippen Method
mcvol	221.150	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1797.50		NIST Webbook
tb	744.17	K	Joback Method
tc	946.14	K	Joback Method
tf	411.38	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.57	J/mol×K	744.17	Joback Method
cpg	646.19	J/mol×K	777.83	Joback Method
cpg	659.85	J/mol×K	811.49	Joback Method
cpg	672.56	J/mol×K	845.16	Joback Method
cpg	684.30	J/mol×K	878.82	Joback Method
cpg	695.08	J/mol×K	912.48	Joback Method
cpg	704.89	J/mol×K	946.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502255&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