D-Methionine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C13H25NO4S/c1-6-17-13(16)14-11(7-8-19-5)12(15)18-10(4)9(2)3/h9-11H,6-8H

InchiKey: MICKYEAKDKWODH-NFJWQWPMSA-N

Formula: C13H25NO4S

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

Mol. weight [g/mol]: 291.41

Physical Properties

Property code	Value	Unit	Source
gf	-294.07	kJ/mol	Joback Method
hf	-721.75	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.442		Crippen Method
mcvol	235.240	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1904.70		NIST Webbook
rinpol	1904.70		NIST Webbook
tb	767.05	K	Joback Method
tc	967.58	K	Joback Method
tf	422.65	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.93	J/mol×K	767.05	Joback Method
cpg	701.87	J/mol×K	800.47	Joback Method
cpg	715.80	J/mol×K	833.89	Joback Method
cpg	728.72	J/mol×K	867.32	Joback Method
cpg	740.65	J/mol×K	900.74	Joback Method
cpg	751.57	J/mol×K	934.16	Joback Method
cpg	761.49	J/mol×K	967.58	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=R501881&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