

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

Inchi:	InChI=1S/C14H27NO4S/c1-6-18-14(17)15-12(8-9-20-7-2)13(16)19-11(5)10(3)4/h10-12H
InchiKey:	WJFMXOHGTNBCRA-JHJMLUEUSA-N
Formula:	C14H27NO4S
SMILES:	CCOC(=O)NC(CCSCC)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	305.43

Physical Properties

Property code	Value	Unit	Source
gf	-285.65	kJ/mol	Joback Method
hf	-742.39	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.832		Crippen Method
mvol	249.330	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1971.70		NIST Webbook
tb	789.93	K	Joback Method
tc	989.57	K	Joback Method
tf	433.92	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.32	J/molxK	789.93	Joback Method
cpg	758.52	J/molxK	823.20	Joback Method
cpg	772.67	J/molxK	856.48	Joback Method
cpg	785.77	J/molxK	889.75	Joback Method
cpg	797.83	J/molxK	923.02	Joback Method
cpg	808.85	J/molxK	956.30	Joback Method
cpg	818.82	J/molxK	989.57	Joback Method

Sources

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=R501821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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