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

Inchi: InChI=1S/C14H26N2O6/c1-6-20-13(18)15-8-11(16-14(19)21-7-2)12(17)22-10(5)9(3)4/h9
InchiKey: ZLFYCFGTMSWVQQ-NFJWQWPMSA-N
Formula: C14H26N2O6
SMILES: CCOC(=O)NCC(NC(=O)OCC)C(=O)OC(C)C(C)C
Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	-463.30	kJ/mol	Joback Method
hf	-975.59	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.435		Crippen Method
mcvol	250.400	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	2029.50		NIST Webbook
rinpol	2029.50		NIST Webbook
tb	847.61	K	Joback Method
tc	1046.47	K	Joback Method
tf	524.34	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.80	J/mol×K	847.61	Joback Method
cpg	800.25	J/mol×K	880.75	Joback Method
cpg	812.61	J/mol×K	913.90	Joback Method
cpg	823.86	J/mol×K	947.04	Joback Method
cpg	834.01	J/mol×K	980.19	Joback Method
cpg	843.06	J/mol×K	1013.33	Joback Method
cpg	850.99	J/mol×K	1046.47	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=R502017&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