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

Inchi: InChI=1S/C17H32N2O6/c1-8-23-17(22)19-14(15(20)24-12(6)10(2)3)9-18-16(21)25-13(7)11(4)5/h10-14H,8-9H2,1-7H3,(H,18,21)(H,19,22)/t12-,13-,14+/m0/s1

InchiKey: AEQVIJQDQPWIID-ZFXTZCCVSA-N

Formula: C17H32N2O6

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

Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
gf	-442.92	kJ/mol	Joback Method
hf	-1048.07	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.459		Crippen Method
mcvol	292.670	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2022.20		NIST Webbook
tb	915.37	K	Joback Method
tc	1122.94	K	Joback Method
tf	528.15	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.27	J/mol×K	915.37	Joback Method
cpg	977.39	J/mol×K	949.96	Joback Method
cpg	990.15	J/mol×K	984.56	Joback Method
cpg	1001.54	J/mol×K	1019.15	Joback Method
cpg	1011.56	J/mol×K	1053.75	Joback Method
cpg	1020.23	J/mol×K	1088.34	Joback Method
cpg	1027.53	J/mol×K	1122.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501767&Units=SI

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