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

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

InchiKey: GKTOTRKMGWTYSG-KWCCSABGSA-N

Formula: C17H32N2O6

SMILES: CCOC(=O)NCCCCC(NC(=O)OCC)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
gf	-438.04	kJ/mol	Joback Method
hf	-1037.51	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.605		Crippen Method
mcvol	292.670	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2373.90		NIST Webbook
tb	916.25	K	Joback Method
tc	1122.68	K	Joback Method
tf	558.15	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.30	J/mol×K	916.25	Joback Method
cpg	976.41	J/mol×K	950.65	Joback Method
cpg	989.19	J/mol×K	985.06	Joback Method
cpg	1000.64	J/mol×K	1019.46	Joback Method
cpg	1010.76	J/mol×K	1053.87	Joback Method
cpg	1019.56	J/mol×K	1088.27	Joback Method
cpg	1027.04	J/mol×K	1122.68	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=R501876&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