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

Inchi: InChI=1S/C16H30N2O6/c1-6-22-15(20)17-10-8-9-13(18-16(21)23-7-2)14(19)24-12(5)11(

InchiKey: PKDJRCOUQAURDP-PZORYLMUSA-N

Formula: C16H30N2O6

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

Mol. weight [g/mol]: 346.42

Physical Properties

Property code	Value	Unit	Source
gf	-446.46	kJ/mol	Joback Method
hf	-1016.87	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.215		Crippen Method
mcvol	278.580	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2271.80		NIST Webbook
tb	893.37	K	Joback Method
tc	1096.44	K	Joback Method
tf	546.88	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.14	J/mol×K	893.37	Joback Method
cpg	917.05	J/mol×K	927.22	Joback Method
cpg	929.71	J/mol×K	961.06	Joback Method
cpg	941.12	J/mol×K	994.91	Joback Method
cpg	951.30	J/mol×K	1028.75	Joback Method
cpg	960.22	J/mol×K	1062.60	Joback Method
cpg	967.91	J/mol×K	1096.44	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=R501910&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