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

Inchi: InChI=1S/C18H33NO6/c1-8-23-18(22)19-15(17(21)25-14(7)12(4)5)9-10-16(20)24-13(6)11(2)3

InchiKey: QOBXCSPBRMIZOJ-GRKKQISMSA-N

Formula: C18H33NO6

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

Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
gf	-523.89	kJ/mol	Joback Method
hf	-1122.18	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.057		Crippen Method
mcvol	296.780	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2148.70		NIST Webbook
tb	888.08	K	Joback Method
tc	1090.76	K	Joback Method
tf	486.76	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.55	J/mol×K	888.08	Joback Method
cpg	979.82	J/mol×K	921.86	Joback Method
cpg	993.77	J/mol×K	955.64	Joback Method
cpg	1006.41	J/mol×K	989.42	Joback Method
cpg	1017.75	J/mol×K	1023.20	Joback Method
cpg	1027.77	J/mol×K	1056.98	Joback Method
cpg	1036.50	J/mol×K	1090.76	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=R502082&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