D-«alpha»-Aminobutyric acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C12H23NO4/c1-6-10(13-12(15)16-7-2)11(14)17-9(5)8(3)4/h8-10H,6-7H2,1-5H3

InchiKey: ZHTVAOXHQKTVHZ-VHMJZVADSA-N

Formula: C12H23NO4

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

Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	-335.61	kJ/mol	Joback Method
hf	-742.98	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.099		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1532.70		NIST Webbook
rinpol	1532.70		NIST Webbook
tb	675.39	K	Joback Method
tc	863.40	K	Joback Method
tf	376.98	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.09	J/mol×K	675.39	Joback Method
cpg	588.21	J/mol×K	706.72	Joback Method
cpg	602.55	J/mol×K	738.06	Joback Method
cpg	616.10	J/mol×K	769.39	Joback Method
cpg	628.87	J/mol×K	800.73	Joback Method
cpg	640.87	J/mol×K	832.06	Joback Method
cpg	652.08	J/mol×K	863.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501752&Units=SI
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

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