

«beta»-Aminoisobutyric acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

InChI=1S/C12H23NO4/c116-16-12(15)13-7-9(4)11(14)17-10(5)8(2)3/h8-10H,6-7H2,1-5H
InChIKey: FFXZTIJHVQTSIA-QVDDQXJPCSA-N

Formula: C12H23NO4
SMILES: CCOC(=O)NCC(C)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	-2.37		Crippen Method
logp	1.956		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1579.10		NIST Webbook
rinpol	1571.00		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/molxK	675.39	Joback Method
cpg	588.21	J/molxK	706.72	Joback Method
cpg	602.55	J/molxK	738.06	Joback Method
cpg	616.10	J/molxK	769.39	Joback Method
cpg	628.87	J/molxK	800.73	Joback Method
cpg	640.87	J/molxK	832.06	Joback Method
cpg	652.08	J/molxK	863.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R501712&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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