

«gamma»-Aminobutyric acid, N-isobutoxycarbonyl-, butyl ester

Other names: .gama.-Aminobutyric acid, N-isobutoxycarbonyl-, butyl ester

Inchi: InChI=1S/C13H25NO4/c1-4-5-9-17-12(15)7-6-8-14-13(16)18-10-11(2)3/h11H,4-10H2,1-3

InchiKey: WYRDREZDCJGYHK-UHFFFAOYSA-N

Formula: C13H25NO4

SMILES: CCCOC(=O)CCCNC(=O)OCC(C)C

Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-322.31	kJ/mol	Joback Method
hf	-753.06	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.492		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
tb	699.15	K	Joback Method
tc	881.01	K	Joback Method
tf	418.25	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.17	J/molxK	699.15	Joback Method
cpg	641.27	J/molxK	729.46	Joback Method
cpg	655.61	J/molxK	759.77	Joback Method
cpg	669.18	J/molxK	790.08	Joback Method
cpg	681.98	J/molxK	820.39	Joback Method
cpg	694.03	J/molxK	850.70	Joback Method
cpg	705.33	J/molxK	881.01	Joback Method

Sources

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=U321047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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