

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

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

Inchi: InChI=1S/C23H45NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-27-22(25)17-16-18-24-23(2

InchiKey: ZFEUCJNQPMYNLE-UHFFFAOYSA-N

Formula: C23H45NO4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCN=C(O)OCC(C)C

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
hf	-980.15	kJ/mol	Joback Method
hvap	98.04	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.598		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	866.58	kPa	Joback Method
tb	992.65	K	Joback Method
tc	1224.98	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321056&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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