

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

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

Inchi: InChI=1S/C20H39NO4/c1-4-5-6-7-8-9-10-11-12-16-24-19(22)14-13-15-21-20(23)25-17-1

InchiKey: ZFQHERUDHUPAOH-UHFFFAOYSA-N

Formula: C20H39NO4

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

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
hf	-918.23	kJ/mol	Joback Method
hvap	91.36	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.427		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	924.01	K	Joback Method
tc	1132.03	K	Joback Method

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321054&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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