

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

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

Inchi: InChI=1S/C25H49NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-29-24(27)19-18-20-2

InchiKey: QNHQUHQEKLJETK-UHFFFAOYSA-N

Formula: C25H49NO4

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

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
hf	-1021.43	kJ/mol	Joback Method
hvap	102.49	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.378		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	776.34	kPa	Joback Method
rinpol	3298.00		NIST Webbook
rinpol	3298.00		NIST Webbook
tb	1038.41	K	Joback Method
tc	1293.43	K	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=U321058&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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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