

DL-3-Aminobutanoic acid, N-hexyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C22H43NO4/c1-4-6-8-10-11-12-13-14-16-17-26-21(24)19-20(3)23-22(25)27-18
InchiKey: BMGVIUBJKAHSHN-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCCCCCCCOC(=O)CC(C)N=C(O)OCCCCC
Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
hf	-959.51	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	6.350		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	917.72	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	969.77	K	Joback Method
tc	1192.79	K	Joback Method

Sources

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=U392813&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/95-893-6/DL-3-Aminobutanoic-acid-N-hexyloxycarbonyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-05-02 21:02:23.165326607 +0000 UTC m=+16972992.085903923.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.