

DL-3-Aminobutanoic acid, N-(2-ethylhexyl)oxycarbonyl-, pentadecyl

Inchi:
ester

InChI=1S/C28H55NO4/c1-5-8-10-11-12-13-14-15-16-17-18-19-20-22-32-27(30)23-25(4)

InchiKey:

WKIGYRSFZYBHDZ-UHFFFAOYSA-N

Formula:

C28H55NO4

SMILES:

CCCCCCCCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC

Mol. weight [g/mol]:

469.74

Physical Properties

Property code	Value	Unit	Source
hf	-1088.63	kJ/mol	Joback Method
hvap	108.78	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.546		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	668.04	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1106.61	K	Joback Method
tc	1403.05	K	Joback Method

Sources

Crippen Method:

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

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=U392827&Units=SI>

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

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