

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

Inchi: InChI=1S/C26H51NO4/c1-5-8-10-11-12-13-14-15-16-17-18-20-30-25(28)21-23(4)27-26(2)
InchiKey: DOKJLQKNADCNTB-UHFFFAOYSA-N
Formula: C26H51NO4
SMILES: CCCCCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC
Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
hf	-1047.35	kJ/mol	Joback Method
hvap	104.33	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.766		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	739.63	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	1060.85	K	Joback Method
tc	1326.13	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=U392825&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

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