

1-Aminocyclopentanecarboxylic acid, N-(octyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C21H39NO4/c1-3-5-7-9-10-14-18-26-20(24)22-21(15-11-12-16-21)19(23)25-17
InchiKey: ZIDCUBAIXFBHAZ-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCCCCCCOC(O)=NC1(C(=O)OCCCCC)CCCC1
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-857.87	kJ/mol	Joback Method
hvap	93.08	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.714		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	962.85	K	Joback Method
tc	1178.80	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392563&Units=SI>
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

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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