

1-Aminocyclopentanecarboxylic acid, N-hexyloxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C19H35NO4/c1-4-5-6-9-14-24-18(22)20-19(12-7-8-13-19)17(21)23-15-10-11-1
InchiKey: PJZZVVUFQKLZRW-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCCCCOC(O)=NC1(C(=O)OCCCC(C)C)CCCC1
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
hf	-821.87	kJ/mol	Joback Method
hvap	88.24	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.790		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
tb	916.65	K	Joback Method
tc	1125.09	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392432&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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