

1-Aminocyclopentanecarboxylic acid, N-((1R)-(-)-menthyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C23H41NO4/c1-5-6-7-10-15-27-21(25)23(13-8-9-14-23)24-22(26)28-20-16-18
InchiKey: SFNTXIMXZGWTCH-UHFFFAOYSA-N
Formula: C23H41NO4
SMILES: CCCCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1
Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
hf	-890.79	kJ/mol	Joback Method
hvap	96.96	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.814		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
tb	1018.38	K	Joback Method
tc	1247.49	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392613&Units=SI>
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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