

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

Inchi: InChI=1S/C24H43NO4/c1-5-6-7-8-11-16-28-22(26)24(14-9-10-15-24)25-23(27)29-21-17-13-2
InchiKey: IPZGFGKOVXXNBE-UHFFFAOYSA-N
Formula: C24H43NO4
SMILES: CCCCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1
Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
hf	-911.43	kJ/mol	Joback Method
hvap	99.19	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.204		Crippen Method
mcvol	352.160	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook
tb	1041.26	K	Joback Method
tc	1274.80	K	Joback Method

Sources

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=U392614&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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