

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

InChI=1S/C27H47NO4/c1-17(2)21-11-10-20(6)23(16-21)31-25(29)27(13-7-8-14-27)28-20
InChIKey: PZCGWBLWQBWGOW-UHFFFAOYSA-N

Formula: C27H47NO4

SMILES: CC1CCC(C(C)C)C(OC(O)=NC2(C(=O)OC3CC(C(C)C)CCC3C)CCCC2)C1

Mol. weight [g/mol]: 449.67

Physical Properties

Property code	Value	Unit	Source
hf	-964.99	kJ/mol	Joback Method
hvap	105.29	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.695		Crippen Method
mcvol	383.570	ml/mol	McGowan Method
pc	935.20	kPa	Joback Method
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook
tb	1119.67	K	Joback Method
tc	1370.83	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392621&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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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