

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

Inchi: InChI=1S/C26H47NO4/c1-5-6-7-8-9-10-13-18-30-24(28)26(16-11-12-17-26)27-25(29)31-
InchiKey: QXFJODVUATUIBR-UHFFFAOYSA-N
Formula: C26H47NO4
SMILES: CCCCCCCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1
Mol. weight [g/mol]: 437.66

Physical Properties

Property code	Value	Unit	Source
hf	-952.71	kJ/mol	Joback Method
hvap	103.64	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.984		Crippen Method
mcvol	380.340	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook
tb	1087.02	K	Joback Method
tc	1332.84	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392616&Units=SI>

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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