

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

Inchi: InChI=1S/C21H37NO4/c1-5-6-13-25-19(23)21(11-7-8-12-21)22-20(24)26-18-14-16(4)9-1
InchiKey: DONIFSNPBGTPB-UHFFFAOYSA-N
Formula: C21H37NO4
SMILES: CCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1
Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
hf	-849.51	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	5.034		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	972.62	K	Joback Method
tc	1195.91	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392611&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
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

Latest version available from:

<https://www.cheméo.com/cid/94-662-3/1-Aminocyclopentanecarboxylic-acid-N-1R-menthyloxycarbonyl-butyl-ester.p>

Generated by Cheméo on 2024-04-27 08:48:56.918321209 +0000 UTC m=+16496985.838898522.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.