

1-Aminocyclopentanecarboxylic acid, N-(isobutoxycarbonyl)-, butyl ester

Inchi: InChI=1S/C15H27NO4/c1-4-5-10-19-13(17)15(8-6-7-9-15)16-14(18)20-11-12(2)3/h12H,4
InchiKey: VZJJNEHUHXDGPS-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CCCCOC(=O)C1(N=C(O)OCC(C)C)CCCC1
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
hf	-739.31	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.229		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	825.13	K	Joback Method
tc	1028.66	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392502&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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