

Pipecolic acid, N-isobutoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C15H27NO4/c1-11(2)9-19-14(17)13-7-5-6-8-16(13)15(18)20-10-12(3)4/h11-13
InchiKey: MDOHTOTVKAPQPU-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CC(C)COC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.833		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1866.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393018&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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