

Pipecolylpipecolic acid, N-isobutoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C21H36N2O5/c1-15(2)13-27-20(25)18-10-6-7-11-22(18)19(24)17-9-5-8-12-23
InchiKey: RYOKFHBWCNJNCA-UHFFFAOYSA-N
Formula: C21H36N2O5
SMILES: CC(C)COC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	3.214		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
rinpol	2633.00		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=U393027&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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