

Pipecolylpipecolic acid, N-butoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C21H36N2O5/c1-4-5-14-27-21(26)23-13-9-6-10-17(23)19(24)22-12-8-7-11-18
InchiKey: AAXCFZXGXFSJDU-UHFFFAOYSA-N
Formula: C21H36N2O5
SMILES: CCCCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.358		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
rinpola	2629.00		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=U393064&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
rinpola: Non-polar retention indices

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