

Pipecolylpipecolic acid, N-ethoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C20H34N2O5/c1-3-5-10-15-27-19(24)17-12-7-8-13-21(17)18(23)16-11-6-9-14
InchiKey: XWZGEEUTMORDQU-UHFFFAOYSA-N
Formula: C20H34N2O5
SMILES: CCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 382.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.112		Crippen Method
mcvol	307.350	ml/mol	McGowan Method
rinpol	2681.00		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=U393083&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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