

Pipecolylpipecolic acid, N-propoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C23H40N2O5/c1-3-5-6-7-12-18-29-22(27)20-14-9-10-15-24(20)21(26)19-13-8
InchiKey: OCYNYIADDRJZMX-UHFFFAOYSA-N
Formula: C₂₃H₄₀N₂O₅
SMILES: CCCCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCC
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.282		Crippen Method
mcvol	349.620	ml/mol	McGowan Method
rinpola	2939.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U393013&Units=SI>

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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