

Pipecolylpipecolic acid, N-hexyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C25H44N2O5/c1-3-5-7-13-19-31-24(29)22-16-10-11-17-26(22)23(28)21-15-9-
InchiKey: MCYNUHDWWQKFOF-UHFFFAOYSA-N
Formula: C25H44N2O5
SMILES: CCCCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCCCC
Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	5.062		Crippen Method
mcvol	377.800	ml/mol	McGowan Method
rinpole	3159.00		NIST Webbook
rinpole	3159.00		NIST Webbook

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=U393123&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
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/118-975-9/Pipecolylpipecolic-acid-N-hexyloxycarbonyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-28 00:07:15.397157846 +0000 UTC m=+16552084.317735160.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.