

Pipecolylpipecolic acid, N-butoxycarbonyl-, decyl ester

Inchi: InChI=1S/C27H48N2O5/c1-3-5-7-8-9-10-11-16-22-33-26(31)24-18-13-14-19-28(24)25(30)27-2
InchiKey: JRPMJQHEKOQDIS-UHFFFAOYSA-N
Formula: C27H48N2O5
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 480.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.843		Crippen Method
mcvol	405.980	ml/mol	McGowan Method
rinpol	3317.00		NIST Webbook
rinpol	3317.00		NIST Webbook

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=U393071&Units=SI>

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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