

Pipecolic acid, N-octyloxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C27H51NO4/c1-3-5-7-9-11-12-13-14-16-19-23-31-26(29)25-21-17-18-22-28(2)
InchiKey: XPSQYYPGSCUOJF-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	7.802		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393133&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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