

Pipecolic acid, N-octyloxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C28H53NO4/c1-3-5-7-9-11-12-13-14-15-17-20-24-32-27(30)26-22-18-19-23-29
InchiKey: NLQRDKQDVRYRRO-UHFFFAOYSA-N
Formula: C28H53NO4
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	8.192		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
rinpole	3257.00		NIST Webbook
rinpole	3257.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393134&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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