

Pipecolic acid, N-octyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C24H45NO4/c1-3-5-7-9-11-13-16-20-28-23(26)22-18-14-15-19-25(22)24(27)29
InchiKey: WLLNYWGFHAHNDU-UHFFFAOYSA-N
Formula: C₂₄H₄₅NO₄
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	6.632		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinpol	2840.00		NIST Webbook
rinpol	2840.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393130&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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