

Pipecolic acid, N-octyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C23H43NO4/c1-3-5-7-9-11-15-19-27-22(25)21-17-13-14-18-24(21)23(26)28-20
InchiKey: LASKFZJULSTHDD-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	6.242		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
rinpole	2741.00		NIST Webbook
rinpole	2741.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393129&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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