

Pipecolic acid, N-isobutoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C23H43NO4/c1-4-5-6-7-8-9-10-11-12-15-18-27-22(25)21-16-13-14-17-24(21)2
InchiKey: GHLIKCZOAYALEJ-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	6.098		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
rinpol	2721.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.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=U393024&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/99-057-0/Pipecolic-acid-N-isobutoxycarbonyl-dodecyl-ester.pdf>

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