

4-Methylvaleric acid, picolinyl ester

Inchi: InChI=1S/C12H17NO2/c1-10(2)5-6-12(14)15-9-11-4-3-7-13-8-11/h3-4,7-8,10H,5-6,9H2,1
InchiKey: BTZVIEPPMAHNOJ-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CC(C)CCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.561		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
rinpol	1603.40		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=U333115&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/85-586-8/4-Methylvaleric-acid-picolinyl-ester.pdf>

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