

Pipecolic acid, N-propoxycarbonyl-, decyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-5-6-7-8-9-10-13-17-24-19(22)18-14-11-12-15-21(18)20(23)2
InchiKey: KQZBOPGDQWRAGP-UHFFFAOYSA-N
Formula: C20H37NO4
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	5.071		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
rinpole	2467.00		NIST Webbook
rinpole	2467.00		NIST Webbook

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=U393001&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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/98-120-0/Pipecolic-acid-N-propoxycarbonyl-decyl-ester.pdf>

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