

2,6-Pyridinedicarboxylic acid, hexyl 2-methylpentyl ester

Inchi: InChI=1S/C19H29NO4/c1-4-6-7-8-13-23-18(21)16-11-9-12-17(20-16)19(22)24-14-15(3)1
InchiKey: KVCKVLMQPMEAQI-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(C)CCC)n1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	4.412		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369086&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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