

2,6-Pyridinedicarboxylic acid, heptyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C25H41NO5/c1-4-6-8-10-12-20-30-24(27)22-17-13-18-23(26-22)25(28)31-21(29)30
InchiKey: YIIPDJKSHFZAHB-UHFFFAOYSA-N
Formula: C₂₅H₄₁NO₅
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(CCCCC)CCCOC)n1
Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.62		Crippen Method
logp	6.131		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369248&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

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