

2,6-Pyridinedicarboxylic acid, hexyl tridecyl ester

Inchi:	InChI=1S/C26H43NO4/c1-3-5-7-9-10-11-12-13-14-15-17-22-31-26(29)24-20-18-19-23(27)
InchiKey:	NEZFOPKCCUYVLM-UHFFFAOYSA-N
Formula:	C26H43NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1
Mol. weight [g/mol]:	433.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.84		Crippen Method
logp	7.287		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
rinsol	3092.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368781&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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