

2,6-Pyridinedicarboxylic acid, 4-chlorobenzyl ethyl ester

Inchi:	InChI=1S/C16H14ClNO4/c1-2-21-15(19)13-4-3-5-14(18-13)16(20)22-10-11-6-8-12(17)9-
InchiKey:	FQVJCROKXKUOBN-UHFFFAOYSA-N
Formula:	C16H14ClNO4
SMILES:	CCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]:	319.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	3.269		Crippen Method
mcvol	225.880	ml/mol	McGowan Method
rinpola	2514.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369135&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
rinpola:	Non-polar retention indices

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