

# 2,6-Pyridinedicarboxylic acid, 3,5-dichlorobenzyl octyl ester

Inchi:	InChI=1S/C22H25Cl2NO4/c1-2-3-4-5-6-7-11-28-21(26)19-9-8-10-20(25-19)22(27)29-15-
InchiKey:	YEXSNDDYQQYEKS-UHFFFAOYSA-N
Formula:	C22H25Cl2NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1
Mol. weight [g/mol]:	438.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.13		Crippen Method
logp	6.263		Crippen Method
mcvol	322.660	ml/mol	McGowan Method
rinpola	3137.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369107&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369107&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## 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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