

2,6-Pyridinedicarboxylic acid, butyl 3,5-dichlorobenzyl ester

Inchi: InChI=1S/C18H17Cl2NO4/c1-2-3-7-24-17(22)15-5-4-6-16(21-15)18(23)25-11-12-8-13(19)
InchiKey: OGLPKOINLDSECB-UHFFFAOYSA-N
Formula: C18H17Cl2NO4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1
Mol. weight [g/mol]: 382.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	4.702		Crippen Method
mcvol	266.300	ml/mol	McGowan Method
rinpol	2833.00		NIST Webbook
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Sources

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=U369104&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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