

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

Inchi: InChI=1S/C18H17Cl2NO4/c1-11(2)9-24-17(22)15-4-3-5-16(21-15)18(23)25-10-12-6-13(14)
InchiKey: TYZIMJITEYXHFD-UHFFFAOYSA-N
Formula: C18H17Cl2NO4
SMILES: CC(C)COC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1
Mol. weight [g/mol]: 382.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.22		Crippen Method
logp	4.558		Crippen Method
mcvol	266.300	ml/mol	McGowan Method
rinpola	2776.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369103&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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