

2,6-Pyridinedicarboxylic acid, 4-bromo-2-methoxybenzyl pentyl ester

Inchi: InChI=1S/C20H22BrNO5/c1-3-4-5-11-26-19(23)16-7-6-8-17(22-16)20(24)27-13-14-9-10-
InchiKey: AVHANJNSCZQHOQ-UHFFFAOYSA-N
Formula: C20H22BrNO5
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Br)cc2OC)n1
Mol. weight [g/mol]: 436.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	4.557		Crippen Method
mcvol	293.370	ml/mol	McGowan Method
rinpola	3060.00		NIST Webbook

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=U369168&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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