

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

Inchi: InChI=1S/C17H16BrNO5/c1-3-23-16(20)13-5-4-6-14(19-13)17(21)24-10-11-7-8-12(18)9-
InchiKey: SVWSOOFMJHVKHH-UHFFFAOYSA-N
Formula: C17H16BrNO5
SMILES: CCOC(=O)c1cccc(C(=O)OCc2ccc(Br)cc2OC)n1
Mol. weight [g/mol]: 394.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	3.386		Crippen Method
mcvol	251.100	ml/mol	McGowan Method
rinpol	2833.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U369167&Units=SI>

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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