Pyridine-2-carboxylic acid, 4-bromo-2-methoxybenzyl ester

Inchi: InChI=1S/C14H12BrNO3/c1-18-13-8-11(15)6-5-10(13)9-19-14(17)12-4-2-3-7-16-12/h2-8

InchiKey: MCDZJWILRSMOBL-UHFFFAOYSA-N

Formula: C14H12BrNO3

SMILES: COc1cc(Br)ccc1COC(=O)c1ccccn1

Mol. weight [g/mol]: 322.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	3.210		Crippen Method
mcvol	201.390	ml/mol	McGowan Method
rinpol	2416.00		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=U369169&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