

6-Hydroxynicotinic acid di-methyl derivative

Other names:	Methyl 6-methoxynicotinate 6-Hydroxynicotinic acid, methyl ether, methyl ester Nicotinic acid, 6-methoxy-, methyl ester 3-Pyridinecarboxylic acid, 6-methoxy-, methyl ester 6-Methoxynicotinic acid methylester
Inchi:	InChI=1S/C8H9NO3/c1-11-7-4-3-6(5-9-7)8(10)12-2/h3-5H,1-2H3
InchiKey:	OVLDWZNVBDRZNN-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	<chem>COC(=O)c1ccc(OC)nc1</chem>
Mol. weight [g/mol]:	167.16
CAS:	26218-80-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	0.877		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
rinsol	1582.80		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=C26218804&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

rinpol: Non-polar retention indices

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