4-Methoxycoumarin

Other names:	2(1H)-Benzopyran-2-one, 4-methoxy
	4-Hydroxycoumarin, methyl ether
	Coumarin, 4-methoxy-
Inchi:	InChI=1S/C10H8O3/c1-12-9-6-10(11)13-8-5-3-2-4-7(8)9/h2-6H,1H3
InchiKey:	MLCMXDYMSAZNPC-UHFFFAOYSA-N
Formula:	C10H8O3
SMILES:	COc1cc(=O)oc2ccccc12
Mol. weight [g/mol]:	176.17
CAS:	20280-81-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.55		Crippen Method
logp	1.802		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
rinpol	1844.00		NIST Webbook
rinpol	1789.20		NIST Webbook
rinpol	1789.20		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=C20280813&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