

Coumarin-d6

Inchi:	InChI=1S/C9H6O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-6H/i1D,2D,3D,4D,5D,6D
InchiKey:	ZYGHJZDHTFUPRJ-MZWXYZOWSA-N
Formula:	C9D6O2
SMILES:	O=c1ccc2ccccc2o1
Mol. weight [g/mol]:	152.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	1.793		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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