7-Chlorocoumarin

Inchi: InChI=1S/C9H5ClO2/c10-7-3-1-6-2-4-9(11)12-8(6)5-7/h1-5H
InchiKey: BWPNKJCEDYRUCB-UHFFFAOYSA-N
Formula: C9H5ClO2
SMILES: O=c1ccc2ccc(Cl)cc2o1
Mol. weight [g/mol]: 180.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.446		Crippen Method
mcvol	118.430	ml/mol	McGowan Method
rinpol	1586.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1586.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R274292&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices