6-Chlorocoumarin

Inchi:	InChI=1S/C9H5ClO2/c10-7-2-3-8-6(5-7)1-4-9(11)12-8/h1-5H
InchiKey:	AMQSYJCKXPUEDR-UHFFFAOYSA-N
Formula:	C9H5ClO2
SMILES:	O=c1ccc2cc(Cl)ccc2o1
Mol. weight [g/mol]:	180.59
CAS:	2051-59-4

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	1578.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1652.00		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=C2051594&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

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