

Coumarin, 4-chloro-7-diethylamino-

Inchi:	InChI=1S/C13H14ClNO2/c1-3-15(4-2)9-5-6-10-11(14)8-13(16)17-12(10)7-9/h5-8H,3-4H2
InchiKey:	RNVTULXTDSCADN-UHFFFAOYSA-N
Formula:	C13H14ClNO2
SMILES:	CCN(CC)c1ccc2c(Cl)cc(=O)oc2c1
Mol. weight [g/mol]:	251.71
CAS:	131447-40-0

Physical Properties

Property code	Value	Unit	Source
ie	7.51	eV	NIST Webbook
log10ws	-7.86		Crippen Method
logp	3.293		Crippen Method
mcvol	184.770	ml/mol	McGowan Method

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=C131447400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/114-530-6/Coumarin-4-chloro-7-diethylamino.pdf>

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