Coumarin, 3-chloro-7-diethylamino-

Inchi: InChI=1S/C13H14ClNO2/c1-3-15(4-2)10-6-5-9-7-11(14)13(16)17-12(9)8-10/h5-8H,3-4H2
InchiKey: CZUSPFIQJDLTQE-UHFFFAOYSA-N
Formula: C13H14ClNO2
SMILES: CCN(CC)c1ccc2cc(Cl)c(=O)oc2c1
Mol. weight [g/mol]: 251.71
CAS: 133590-12-2

Physical Properties

Property code	Value	Unit	Source
ie	7.53	eV	NIST Webbook
log10ws	-7.86		Crippen Method
logp	3.293		Crippen Method
mcvol	184.770	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=C133590122&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.