

6,8-Dichlorochromone-3-carboxaldehyde

Inchi:	InChI=1S/C10H4Cl2O3/c11-6-1-7-9(14)5(3-13)4-15-10(7)8(12)2-6/h1-4H
InchiKey:	IHCCHRKNCOFDAJ-UHFFFAOYSA-N
Formula:	C10H4Cl2O3
SMILES:	O=Cc1coc2c(Cl)cc(Cl)cc2c1=O
Mol. weight [g/mol]:	243.04
CAS:	64481-11-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	2.912		Crippen Method
mcvol	146.330	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=C64481114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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