

Chromone-3-carbonitrile

Inchi:	InChI=1S/C10H5NO2/c11-5-7-6-13-9-4-2-1-3-8(9)10(7)12/h1-4,6H
InchiKey:	SFWNPLLGXKJESA-UHFFFAOYSA-N
Formula:	C10H5NO2
SMILES:	N#Cc1coc2ccccc2c1=O
Mol. weight [g/mol]:	171.15
CAS:	50743-17-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	1.665		Crippen Method
mcvol	121.660	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=C50743174&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

Latest version available from:

<https://www.chemeo.com/cid/90-996-7/Chromone-3-carbonitrile.pdf>

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