6-Formaldehydecoumarin

Inchi: InChI=1S/C10H6O3/c11-6-7-1-3-9-8(5-7)2-4-10(12)13-9/h1-6H
InchiKey: RQCHYJGDSCWRSQ-UHFFFAOYSA-N
Formula: C10H6O3
SMILES: O=Cc1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]: 174.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.67		Crippen Method
logp	1.606		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
rinpol	1693.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1770.00		NIST Webbook

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=R274252&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
rinpol: Non-polar retention indices

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