

Dehydronepetalactone

Inchi: InChI=1S/C10H12O2/c1-6-3-4-8-7(2)5-12-10(11)9(6)8/h5-6H,3-4H2,1-2H3
InchiKey: JRMIDKPHJPTJMM-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: Cc1coc(=O)c2c1CCC2C
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.57		Crippen Method
logp	1.998		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinsol	1470.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R44003&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/94-299-7/Dehydronepetalactone.pdf>

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