6-Carboxycoumarin

Inchi: InChI=1S/C10H6O4/c11-9-4-2-6-5-7(10(12)13)1-3-8(6)14-9/h1-5H,(H,12,13)
InchiKey: GEFDYGOYVXEKBE-UHFFFAOYSA-N
Formula: C10H6O4
SMILES: O=C(O)c1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]: 190.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	1.491		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
rinpol	1871.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R274232&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices