2H-1-Benzopyran-2-one, 6-amino-

Other names: Coumarin, 6-amino-
6-Amino-1,2-benzopyrone
6-Aminocoumarin
Inchi: InChI=1S/C9H7NO2/c10-7-2-3-8-6(5-7)1-4-9(11)12-8/h1-5H,10H2
InchiKey: ZOJAINJCZSVZGW-UHFFFAOYSA-N
Formula: C9H7NO2
SMILES: Nc1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]: 161.16
CAS: 14415-44-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	1.375		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
rinpol	1806.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1806.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14415442&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

rinpol: Non-polar retention indices