

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:	<chem>Nc1ccc2oc(=O)ccc2c1</chem>
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/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/41-240-9/2H-1-Benzopyran-2-one-6-amino.pdf>

Generated by Cheméo on 2024-04-25 21:12:28.23019643 +0000 UTC m=+16368797.150773790.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.