

6-Nitrocoumarin

Other names:	2H-1-Benzopyran-2-one, 6-nitro- 6-nitro-2-benzopyrone
Inchi:	InChI=1S/C9H5NO4/c11-9-4-1-6-5-7(10(12)13)2-3-8(6)14-9/h1-5H
InchiKey:	RMERXEXZXIVNBF-UHFFFAOYSA-N
Formula:	C9H5NO4
SMILES:	O=c1ccc2cc([N+](=O)[O-])ccc2o1
Mol. weight [g/mol]:	191.14
CAS:	2725-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	1.701		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	313.44		NIST Webbook
rinpol	313.75		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1875.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2725817&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

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