7-Nitrocoumarin

Inchi: InChI=1S/C9H5NO4/c11-9-4-2-6-1-3-7(10(12)13)5-8(6)14-9/h1-5H
InchiKey: XSECDQPYFOEVPU-UHFFFAOYSA-N
Formula: C9H5NO4
SMILES: O=c1ccc2ccc([N+](=O)[O-])cc2o1
Mol. weight [g/mol]: 191.14

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	1809.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1894.00		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=R274301&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

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