

7-Nitro-3,4-benzocoumarin

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|-----------------------------|--|
| Other names: | 3-Nitro-6H-dibenzo[b,d]pyran-6-one |
| Inchi: | InChI=1S/C13H7NO4/c15-13-11-4-2-1-3-9(11)10-6-5-8(14(16)17)7-12(10)18-13/h1-7H |
| InchiKey: | KWGYGQPIDANWAX-UHFFFAOYSA-N |
| Formula: | C13H7NO4 |
| SMILES: | O=c1oc2cc([N+](=O)[O-])ccc2c2ccccc12 |
| Mol. weight [g/mol]: | 241.20 |
| CAS: | 6638-64-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.89 | | Crippen Method |
| logp | 2.854 | | Crippen Method |
| mcvol | 160.510 | ml/mol | McGowan Method |
| rinpol | 394.97 | | NIST Webbook |
| rinpol | 394.41 | | NIST Webbook |
| rinpol | 391.48 | | NIST Webbook |
| rinpol | 394.97 | | NIST Webbook |
| rinpol | 391.48 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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=C6638648&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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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<https://www.chemeo.com/cid/116-671-8/7-Nitro-3-4-benzocoumarin.pdf>

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