7-Nitro-3,4-benzocoumarin

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