

Norgraveoline

Inchi: InChI=1S/C16H11NO3/c18-14-8-13(17-12-4-2-1-3-11(12)14)10-5-6-15-16(7-10)20-9-19-
InchiKey: XZLHQSQFBBOXIY-UHFFFAOYSA-N
Formula: C16H11NO3
SMILES: O=c1cc(-c2ccc3c(c2)OCO3)[nH]c2ccccc12
Mol. weight [g/mol]: 265.26
CAS: 74054-38-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.73 | | Crippen Method |
| logp | 2.442 | | Crippen Method |
| mcvol | 186.050 | ml/mol | McGowan Method |
| rinpol | 3081.90 | | NIST Webbook |
| rinpol | 3081.90 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C74054389&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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<https://www.chemeo.com/cid/124-250-6/Norgraveoline.pdf>

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