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
logp	2.442		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
rinpol	3081.90		NIST Webbook
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Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74054389&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/124-250-6/Norgraveoline.pdf

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