

Isocorydine

Inchi: InChI=1S/C20H23NO4/c1-21-8-7-12-10-15(24-3)20(25-4)18-16(12)13(21)9-11-5-6-14(23)
InchiKey: QELDJEKNFOQJOY-UHFFFAOYSA-N
Formula: C20H23NO4
SMILES: COc1ccc2c(c1O)-c1c(OC)c(OC)cc3c1C(C2)N(C)CC3
Mol. weight [g/mol]: 341.40
CAS: 475-67-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.170		Crippen Method
mcvol	256.880	ml/mol	McGowan Method
rinpol	2913.60		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C475672&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

Latest version available from:

<https://www.chemeo.com/cid/96-473-1/Isocorydine.pdf>

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