

(E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(pyrrolidin-1-yl)n

Inchi: InChI=1S/C20H27NO3/c22-20(21-13-7-8-14-21)10-6-4-2-1-3-5-9-17-11-12-18-19(15-17)
InchiKey: VBHDFZGBKBFFDM-WEV VVXLNSA-N
Formula: C20H27NO3
SMILES: O=C(CCCCCC=Cc1ccc2c(c1)OCO2)N1CCCC1
Mol. weight [g/mol]: 329.43
CAS: 62510-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	4.392		Crippen Method
mcvol	266.170	ml/mol	McGowan Method
rinpol	3100.20		NIST Webbook
rinpol	3100.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C62510525&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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/97-883-5/E-9-Benzo-d-1-3-dioxol-5-yl-1-pyrrolidin-1-yl-non-8-en-1-one.pdf>

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