

(2E,4E,8E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin

Inchi: InChI=1S/C21H25NO3/c23-21(22-14-8-5-9-15-22)11-7-4-2-1-3-6-10-18-12-13-19-20(16-
InchiKey: KAYVDASZRFLFRZ-PQECNABGSA-N
Formula: C21H25NO3
SMILES: O=C(C=CC=CCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 339.43
CAS: 107584-38-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.48 | | Crippen Method |
| logp | 4.334 | | Crippen Method |
| mcvol | 271.660 | ml/mol | McGowan Method |
| rinpol | 3327.70 | | NIST Webbook |
| rinpol | 3327.70 | | 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=C107584383&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/96-289-6/2E-4E-8E-9-Benzo-d-1-3-dioxol-5-yl-1-piperidin-1-yl-nona-2-4-8-trien-1-one.p>

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