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

**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/ci990307l

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices