Omeprazole

Other names: 5-methoxy-2-(((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)sulfinyl)-1H-benzo[d]imidazole
6-methoxy-2-(((4-methoxy-3,5-dimethyl-2-pyridinyl)methyl)sulfinyl)-1H-benzimidazole
Inchi: InChI=1S/C17H19N3O3S/c1-10-8-18-15(11(2)16(10)23-4)9-24(21)17-19-13-6-5-12(22-3)
InchiKey: SUBDBMMJDZJVOS-UHFFFAOYSA-N
Formula: C17H19N3O3S
SMILES: COc1ccc2nc(S(=O)Cc3ncc(C)c(OC)c3C)[nH]c2c1
Mol. weight [g/mol]: 345.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	2.418		Crippen Method
mcvol	251.610	ml/mol	McGowan Method
tf	429.15	K	Thermodynamic models for determination of the solubility of omeprazole in pure and mixture organic solvents from T = (278.15 to 333.15) K

Sources

Thermodynamic models for determination of the solubility of omeprazole in pure and mixture organic solvents from T = (278.15 to 333.15) K: https://www.doi.org/10.1016/j.jct.2015.11.005
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point