

Furosemide-methelute

Other names: Furosemide Me, #1
Inchi: InChI=1S/C15H17ClN2O5S/c1-18(2)24(20,21)14-7-11(15(19)22-3)13(8-12(14)16)17-9-1
InchiKey: FHRXDNPIDVWGNR-UHFFFAOYSA-N
Formula: C15H17ClN2O5S
SMILES: COC(=O)c1cc(S(=O)(=O)N(C)C)c(Cl)cc1NCc1ccc1
Mol. weight [g/mol]: 372.82

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.92 | | Crippen Method |
| logp | 2.582 | | Crippen Method |
| mcvol | 252.590 | ml/mol | McGowan Method |
| rinpol | 2805.00 | | NIST Webbook |
| rinpol | 2805.00 | | 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=U121237&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/121-976-4/Furosemide-methelute.pdf>

Generated by Cheméo on 2024-05-01 05:46:54.433834751 +0000 UTC m=+16831663.354412073.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.