

Clotiazepam M (dihydroxy-), acetylated

Inchi: InChI=1S/C20H19ClN2O5S/c1-5-13-8-14-19(22-9-17(26)23(4)20(14)29-13)18-15(21)6-1
InchiKey: COTLORZBDDVERP-UHFFFAOYSA-N
Formula: C20H19ClN2O5S
SMILES: CCc1cc2c(s1)N(C)C(=O)CN=C2c1c(Cl)cc(OC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 434.89

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.71 | | Crippen Method |
| logp | 3.628 | | Crippen Method |
| mcvol | 299.280 | ml/mol | McGowan Method |
| rinpola | 2995.00 | | NIST Webbook |
| rinpola | 2995.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R312948&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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