

claritine

Other names:

ethyl
4-(8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-ylidene)-1-piperidinec
loratadine

Inchi: InChI=1S/C22H23ClN2O2/c1-2-27-22(26)25-12-9-15(10-13-25)20-19-8-7-18(23)14-17(1**InchiKey:** JCCNYMKQOSZNPW-UHFFFAOYSA-N**Formula:** C22H23ClN2O2**SMILES:** CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc3cccnc32)CC1**Mol. weight [g/mol]:** 382.89

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--|
| hfus | 24.48 | kJ/mol | Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities |
| log10ws | -6.36 | | Crippen Method |
| logp | 4.888 | | Crippen Method |
| mvol | 286.940 | ml/mol | McGowan Method |
| tf | 407.00 | K | Solubility measurement of an antihistamine drug (Loratadine) in supercritical carbon dioxide: Assessment of qCPA and PCP-SAFT equations of state |
| tt | 305.40 | K | Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities |
| tt | 410.00 | K | Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities |

Sources

Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between dynamic and thermodynamic fragilities: <https://www.doi.org/10.1016/j.tca.2018.03.012>
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
Solubility measurement of an antihistamine drug (Loratadine) in supercritical carbon dioxide: Assessment of qCPA and PCP-SAFT equations of state: <https://www.doi.org/10.1016/j.fluid.2018.05.018>

Legend

hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point
tt: Triple Point Temperature

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