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(19
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
mcvol	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

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
Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between thermodynamic 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

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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