

Appendix M. Predicted Atmospheric Half-Life Using EPISUITE Version 4.0

SMILES : CCN(CC)C(=O)SCc1ccc(CL)cc1

CHEM :

MOL FOR: C12 H16 CL1 N1 O1 S1

MOL WT : 257.78

----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) -----

Hydrogen Abstraction = 11.8228 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 11.9000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.6711 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 25.3939 E-12 cm3/molecule-sec

HALF-LIFE = 0.421 Days (12-hr day; 1.5E6 OH/cm3)

HALF-LIFE = 5.054 Hrs

..... ** Designates Estimation(s) Using ASSUMED Value(s)

----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----

***** NO OZONE REACTION ESTIMATION *****
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
