Quazepam + M (oxo-), hydrolysis

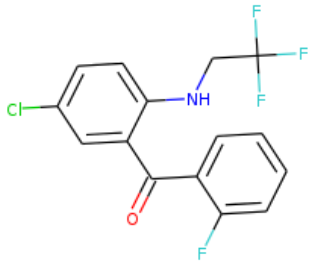
InChI: InChI=1S/C15H10ClF4NO/c16-9-5-6-13(21-8-15(18,19)20)11(7-9)14(22)10-3-1-2-4-12(10)17/h1-7,21H,8H2

InChI Key: VGNVFAXJHFXDAT-UHFFFAOYSA-N

Formula: C15H10ClF4NO

SMILES: O=C(c1ccccc1F)c1cc(Cl)ccc1NCC(F)(F)F

Molecular Weight: 331.69



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-556.51	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-782.32	kJ/mol	Joback Method
$\Delta_{fus} H°$	37.32	kJ/mol	Joback Method
$\Delta_{vap} H°$	68.53	kJ/mol	Joback Method
$logP_{oct/wat}$	4.68		Crippen Method
P_c	2137.41	kPa	Joback Method
T_{boil}	746.22	K	Joback Method
T_c	963.44	K	Joback Method
T_{fus}	486.50	K	Joback Method
V_c	0.81	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	547.76	J/mol×K	746.22	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H10ClF4NO/c16-9-5-6-13(21-8-15(18,19)20)11(7-9)14(22)10-3-1-2-4-12(10)17/h1-7,21H,8H2

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).

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