5-Chloro-2-methylaniline, N,N-bis(pentafluoropropionyl)-

Other names: N-(5-Chloro-2-methylphenyl)-N-(2,2,3,3,3-pentafluoropropanoyl)-2,2,3,3,3-pentafluoropropanamide.

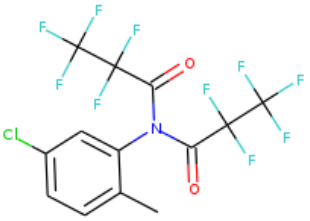
InChI: InChI=1S/C13H6ClF10NO2/c1-5-2-3-6(14)4-7(5)25(8(26)10(15,16)12(19,20)21)9(27)11(17,18)13(22,23)24/h2-4H,1H3

InChI Key: DBEZOKYQVJEFTL-UHFFFAOYSA-N

Formula: C13H6ClF10NO2

SMILES: Cc1ccc(Cl)cc1N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F

Molecular Weight: 433.63



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1944.00	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-2267.53	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	54.70	kJ/mol	Joback Method
$logP_{oct/wat}$	4.90		Crippen Method
P_c	1663.26	kPa	Joback Method
T_{boil}	670.87	K	Joback Method
T_c	847.81	K	Joback Method
T_{fus}	465.56	K	Joback Method
V_c	0.87	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	591.77	J/mol×K	670.87	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H6ClF10NO2/c1-5-2-3-6(14)4-7(5)25(8(26)10(15,16)12(19,20)21)9(27)11(17,18)13(22,23)24/h2-4H,1H3

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

Legend

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