5-Chloro-2-methyl-aniline, N,N-bis(heptafluorobutyryl)-

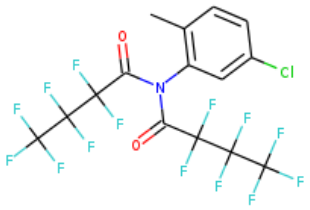
InChI: InChI=1S/C15H6ClF14NO2/c1-5-2-3-6(16)4-7(5)31(8(32)10(17,18)12(21,22)14(25,26)27)9(33)11(19,20)13(23,24)15(28,29)30/h2-4H,1H3

InChI Key: XTWIKYIKGIIDHF-UHFFFAOYSA-N

Formula: C15H6ClF14NO2

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

Molecular Weight: 533.64



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-2700.72	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-3110.75	kJ/mol	Joback Method
$\Delta_{fus} H°$	36.92	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.29	kJ/mol	Joback Method
$logP_{oct/wat}$	6.17		Crippen Method
P_c	1288.36	kPa	Joback Method
T_{boil}	707.25	K	Joback Method
T_c	877.02	K	Joback Method
T_{fus}	495.30	K	Joback Method
V_c	1.03	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	731.25	J/mol×K	707.25	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H6ClF14NO2/c1-5-2-3-6(16)4-7(5)31(8(32)10(17,18)12(21,22)14(25,26)27)9(33)11(19,20)13(23,24)15(28,29)30/h2-4H,1H3

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).