2-[Bis(2,2,3,3,4,4,4-heptafluorobutanoyl)amino]phenyl heptafluorobutanoate

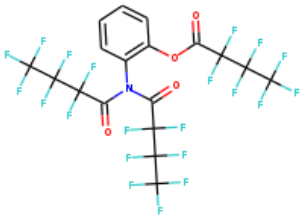
InChI: InChI=1S/C18H4F21NO4/c19-10(20,13(25,26)16(31,32)33)7(41)40(8(42)11(21,22)14(27,28)17(34,35)36)5-3-1-2-4-6(5)44-9(43)12(23,24)15(29,30)18(37,38)39/h1-4H

InChI Key: YGJQDGTZSXQRCE-UHFFFAOYSA-N

Formula: C18H4F21NO4

SMILES: O=C(Oc1ccccc1N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

Molecular Weight: 697.20



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-4242.97	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-4789.28	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.99	kJ/mol	Joback Method
$\Delta_{vap} H°$	54.47	kJ/mol	Joback Method
$logP_{oct/wat}$	6.95		Crippen Method
P_c	956.14	kPa	Joback Method
T_{boil}	794.97	K	Joback Method
T_c	973.74	K	Joback Method
T_{fus}	570.22	K	Joback Method
V_c	1.27	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	964.99	J/mol×K	794.97	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H4F21NO4/c19-10(20,13(25,26)16(31,32)33)7(41)40(8(42)11(21,22)14(27,28)17(34,35)36)5-3-1-2-4-6(5)44-9(43)12(23,24)15(29,30)18(37,38)39/h1-4H

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°$_{gas}$**: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{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).