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

Inchikey: 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

Mol. weight [g/mol]: 697.20

Physical Properties

Property code	Value	Unit	Source
gf	-4242.97	kJ/mol	Joback Method
hf	-4789.28	kJ/mol	Joback Method
hfus	42.99	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	6.950		Crippen Method
mcvol	298.450	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	1221.00		NIST Webbook
tb	794.97	K	Joback Method
tc	973.74	K	Joback Method
tf	570.22	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.99	J/mol×K	794.97	Joback Method
cpg	973.52	J/mol×K	824.77	Joback Method
cpg	981.23	J/mol×K	854.56	Joback Method
cpg	988.24	J/mol×K	884.36	Joback Method
cpg	994.72	J/mol×K	914.15	Joback Method
cpg	1000.80	J/mol×K	943.95	Joback Method
cpg	1006.63	J/mol×K	973.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume