4-(4-Aminophenoxy)aniline, N,N'-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C18H10F10N2O3/c19-15(20,17(23,24)25)13(31)29-9-1-5-11(6-2-9)33-12-7-3-1

InchiKey: QAYGJBSUSLOEFO-UHFFFAOYSA-N

Formula: C18H10F10N2O3

SMILES: O=C(Nc1ccc(Oc2ccc(NC(=O)C(F)(F)C(F)(F)F)cc2)cc1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 492.27

Physical Properties

Property code	Value	Unit	Source
gf	-1814.56	kJ/mol	Joback Method
hf	-2211.27	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	76.96	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.751		Crippen Method
mcvol	263.630	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2247.00		NIST Webbook
tb	884.84	K	Joback Method
tc	1089.85	K	Joback Method
tf	613.49	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.99	J/mol×K	884.84	Joback Method
cpg	833.03	J/mol×K	919.01	Joback Method
cpg	841.34	J/mol×K	953.18	Joback Method
cpg	849.02	J/mol×K	987.34	Joback Method
cpg	856.20	J/mol×K	1021.51	Joback Method
cpg	863.00	J/mol×K	1055.68	Joback Method
cpg	869.53	J/mol×K	1089.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373251&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