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

Inchi: InChI=1S/C21H9F15N2O4/c22-16(23,19(28,29)30)13(39)37-9-1-5-11(6-2-9)42-12-7-3-10

InchiKey: ZZCRBOYHMWDXDH-UHFFFAOYSA-N

Formula: C21H9F15N2O4

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

Mol. weight [g/mol]: 638.28

Physical Properties

Property code	Value	Unit	Source
gf	-2865.20	kJ/mol	Joback Method
hf	-3369.76	kJ/mol	Joback Method
hfus	53.27	kJ/mol	Joback Method
hvap	79.31	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.870		Crippen Method
mcvol	316.320	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2026.00		NIST Webbook
tb	959.51	K	Joback Method
tc	1175.55	K	Joback Method
tf	684.83	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.14	J/mol×K	959.51	Joback Method
cpg	1033.89	J/mol×K	995.52	Joback Method
cpg	1042.22	J/mol×K	1031.52	Joback Method
cpg	1050.33	J/mol×K	1067.53	Joback Method
cpg	1058.42	J/mol×K	1103.54	Joback Method
cpg	1066.69	J/mol×K	1139.55	Joback Method
cpg	1075.34	J/mol×K	1175.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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