4-(4-Aminophenoxy)aniline, N,N,N',N'-tetrakis(trifluoroacetyl)-

Other names: N,N'-(Oxydi-4,1-phenylene)bis[2,2,2-trifluoro-N-(trifluoroacetyl)acetamide]

Inchi: InChI=1S/C20H8F12N2O5/c21-17(22,23)13(35)33(14(36)18(24,25)26)9-1-5-11(6-2-9)39

InchiKey: ILWWKMVSDQWDMU-UHFFFAOYSA-N

Formula: C20H8F12N2O5

SMILES: O=C(N(C(=O)C(F)(F)F)c1ccc(Oc2ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)cc2)cc1)C(F)(F)F

Mol. weight [g/mol]: 584.27

Physical Properties

Property code	Value	Unit	Source
gf	-2402.40	kJ/mol	Joback Method
hf	-2841.81	kJ/mol	Joback Method
hfus	55.79	kJ/mol	Joback Method
hvap	84.48	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.447		Crippen Method
mcvol	298.490	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1863.00		NIST Webbook
rinpol	1863.00		NIST Webbook
tb	961.42	K	Joback Method
tc	1177.06	K	Joback Method
tf	696.69	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.82	J/mol×K	961.42	Joback Method
cpg	948.81	J/mol×K	997.36	Joback Method
cpg	956.23	J/mol×K	1033.30	Joback Method
cpg	963.23	J/mol×K	1069.24	Joback Method
cpg	969.99	J/mol×K	1105.18	Joback Method
cpg	976.65	J/mol×K	1141.12	Joback Method
cpg	983.37	J/mol×K	1177.06	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=U373473&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

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