N-(Trifluoroacetyl)-N-(4-(4-[(trifluoroacetyl)amino]

Other names: 4-(4-Aminophenoxy)aniline, N,N,N'-triskis(trifluoroacetyl)-
N-(Trifluoroacetyl)-N-(4-{4-[(trifluoroacetyl)amino]phenoxy}phenyl)-2,2,2-trifluoroacetamid
Inchi: InChI=1S/C18H9F9N2O4/c19-16(20,21)13(30)28-9-1-5-11(6-2-9)33-12-7-3-10(4-8-12)29
InchiKey: UOQVFOADCHILQU-UHFFFAOYSA-N
Formula: C18H9F9N2O4
SMILES: O=C(Nc1ccc(Oc2ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)cc2)cc1)C(F)(F)F
Mol. weight [g/mol]: 488.26

Physical Properties

Property code	Value	Unit	Source
gf	-1730.12	kJ/mol	Joback Method
hf	-2104.93	kJ/mol	Joback Method
hfus	49.26	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.964		Crippen Method
mcvol	263.430	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	904.94	K	Joback Method
tc	1113.22	K	Joback Method
tf	640.22	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.80	J/mol×K	904.94	Joback Method
cpg	820.30	J/mol×K	939.65	Joback Method
cpg	828.05	J/mol×K	974.37	Joback Method
cpg	835.15	J/mol×K	1009.08	Joback Method
cpg	841.73	J/mol×K	1043.80	Joback Method
cpg	847.89	J/mol×K	1078.51	Joback Method

cpg	853.73	J/mol×K	1113.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373342&Units=SI

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