2-(Bis(trifluoroacetyl)amino)phenyl trifluoroacetate

Other names: o-Aminophenol, N,N,O-tris(trifluoroacetyl)-
Inchi: InChI=1S/C12H4F9NO4/c13-10(14,15)7(23)22(8(24)11(16,17)18)5-3-1-2-4-6(5)26-9(25)
InchiKey: AKOGAMFZGCLQDM-UHFFFAOYSA-N
Formula: C12H4F9NO4
SMILES: O=C(Oc1ccccc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 397.15

Physical Properties

Property code	Value	Unit	Source
gf	-1972.81	kJ/mol	Joback Method
hf	-2259.62	kJ/mol	Joback Method
hfus	34.97	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.139		Crippen Method
mcvol	192.670	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
tb	685.83	K	Joback Method
tc	864.56	K	Joback Method
tf	481.00	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.79	J/mol×K	685.83	Joback Method
cpg	553.81	J/mol×K	715.62	Joback Method
cpg	562.05	J/mol×K	745.41	Joback Method
cpg	569.56	J/mol×K	775.19	Joback Method
cpg	576.39	J/mol×K	804.98	Joback Method
cpg	582.61	J/mol×K	834.77	Joback Method
cpg	588.27	J/mol×K	864.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373274&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

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