Ethanone, 2,2,2-trifluoro-1-phenyl-

Other names:	(Trifluoroacetyl)benzene
	1,1,1-Trifluoroacetophenone
	2,2,2-Trifluoro-1-phenylethanone
	2,2,2-Trifluoroacetophenone
	Acetophenone, 2,2,2-trifluoro-
	NSC 42752
	Phenyl trifluoromethyl ketone
	Trifluoroacetophenone
	Trifluoromethyl phenyl ketone
	alpha,alpha,alpha-Trifluoroacetophenone
	«alpha»,«alpha»,«alpha»-Trifluoroacetophenone
	«omega»,«omega»,«omega»-Trifluoroacetophenone
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoroacetophenone
	Â«omegaÂ»,Â«omegaÂ»,Â«omegaÂ»-Trifluoroacetophenone
Inchi:	InChI=1S/C8H5F3O/c9-8(10,11)7(12)6-4-2-1-3-5-6/h1-5H
InchiKey:	KZJRKRQSDZGHEC-UHFFFAOYSA-N
Formula:	C8H5F3O
SMILES:	O=C(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	174.12
CAS:	434-45-7

Physical Properties

Property code	Value	Unit	Source
affp	799.20	kJ/mol	NIST Webbook
basg	767.40	kJ/mol	NIST Webbook
ea	0.98 ± 0.09	eV	NIST Webbook
gf	-581.62	kJ/mol	Joback Method
hf	-681.58	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	38.68	kJ/mol	Joback Method
ie	10.25	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	10.25	eV	NIST Webbook
log10ws	-1.16		Aqueous Solubility Prediction Method
logp	2.432		Crippen Method
mcvol	106.700	ml/mol	McGowan Method

pc	3427.87	kPa	Joback Method
rinpol	866.00		NIST Webbook
tb	438.50 ± 0.50	K	NIST Webbook
tb	438.70	K	NIST Webbook
tc	658.50	K	Joback Method
tf	233.00 ± 6.00	K	NIST Webbook
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.31	J/mol×K	457.57	Joback Method
cpg	231.49	J/mol×K	491.06	Joback Method
cpg	241.86	J/mol×K	524.55	Joback Method
cpg	251.45	J/mol×K	558.04	Joback Method
cpg	260.30	J/mol×K	591.52	Joback Method
cpg	268.45	J/mol×K	625.01	Joback Method
cpg	275.96	J/mol×K	658.50	Joback Method
hvapt	43.10	kJ/mol	383.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.20	K	97.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67771e+01
Coeff. B	-5.18144e+03
Temperature range (K), min.	314.23
Temperature range (K), max.	451.91

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C434457&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume