1,2,4-Trifluorobenzene

Other names:	1,3,4-trifluorobenzene
	1,4,5-trifluorobenzene
	benzene, 1,2,4-trifluoro-
Inchi:	InChI=1S/C6H3F3/c7-4-1-2-5(8)6(9)3-4/h1-3H
InchiKey:	PEBWOGPSYUIOBP-UHFFFAOYSA-N
Formula:	C6H3F3
SMILES:	Fc1ccc(F)c(F)c1
Mol. weight [g/mol]:	132.08
CAS:	367-23-7

Physical Properties

Property code	Value	Unit	Source
affp	729.50	kJ/mol	NIST Webbook
basg	699.40	kJ/mol	NIST Webbook
gf	-491.64	kJ/mol	Joback Method
hf	-541.91	kJ/mol	Joback Method
hfus	13.80	kJ/mol	Joback Method
hvap	30.10	kJ/mol	Joback Method
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.05	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
log10ws	-2.47		Crippen Method
logp	2.104		Crippen Method
mcvol	76.950	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	363.00 ± 1.00	K	NIST Webbook
tc	553.01	K	Joback Method
tf	210.61	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.86	J/mol×K	492.38	Joback Method

cpg	164.90	J/mol×K	522.70	Joback Method
cpg	131.45	J/mol×K	371.13	Joback Method
cpg	138.81	J/mol×K	401.44	Joback Method
cpg	145.82	J/mol×K	431.76	Joback Method
cpg	152.50	J/mol×K	462.07	Joback Method
cpg	170.64	J/mol×K	553.01	Joback Method
rhol	1280.00	kg/m3	296.60	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1247.00	kg/m3	330.70	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	101.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1021/je8006474
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=C367237&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume