1,2,3-Trifluorobenzene

Other names: benzene, 1,2,3-trifluoro-
Inchi: InChI=1S/C6H3F3/c7-4-2-1-3-5(8)6(4)9/h1-3H
InchiKey: AJKNNUJQFALRIK-UHFFFAOYSA-N
Formula: C6H3F3
SMILES: Fc1cccc(F)c1F
Mol. weight [g/mol]: 132.08
CAS: 1489-53-8

Physical Properties

Property code	Value	Unit	Source
affp	724.30	kJ/mol	NIST Webbook
basg	696.60	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	9.40	eV	NIST Webbook
ie	9.70	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	367.70	K	NIST Webbook
tb	367.50 ± 0.50	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	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	158.86	J/mol×K	492.38	Joback Method
cpg	164.90	J/mol×K	522.70	Joback Method
cpg	170.64	J/mol×K	553.01	Joback Method
rhol	1292.00	kg/m3	296.00	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1240.00	kg/m3	331.60	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

Sources

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=C1489538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume