1,3,5-Trifluorobenzene

Other names:	Benzene, 1,3,5-trifluoro- SYM-TRIFLUOROBENZENE
Inchi:	InChI=1S/C6H3F3/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey:	JXUKFFRPLNTYIV-UHFFFAOYSA-N
Formula:	C6H3F3
SMILES:	Fc1cc(F)cc(F)c1
Mol. weight [g/mol]:	132.08
CAS:	372-38-3

Physical Properties

Property code	Value	Unit	Source
affp	741.90	kJ/mol	NIST Webbook
basg	715.40	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	33.90	kJ/mol	NIST Webbook
hvap	33.74	kJ/mol	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
ie	9.50	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	348.70	K	NIST Webbook
tb	348.60	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
hvapt	34.50	kJ/mol	314.50	NIST Webbook
rhol	1268.00	kg/m3	297.20	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1225.00	kg/m3	324.90	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48636e+01
Coeff. B	-3.18142e+03
Coeff. C	-3.80750e+01
Temperature range (K), min.	256.34
Temperature range (K), max.	371.13

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.06127e+02
Coeff. B	-7.50035e+03
Coeff. C	-1.39799e+01
Coeff. D	1.47070e-05
Temperature range (K), min.	279.15
Temperature range (K), max.	323.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1673.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1673

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
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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature

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