Benzene, 1,3,5-trichloro-2,4,6-trifluoro-

Other names:	1,3,5-TRICHLORO-2,4,6-TRIFLUOROBENZENE
	1,3,5-Trichlorotrifluorobenzene
Inchi:	InChI=1S/C6Cl3F3/c7-1-4(10)2(8)6(12)3(9)5(1)11
InchiKey:	QPXZZPSKCVNHFW-UHFFFAOYSA-N
Formula:	C6Cl3F3
SMILES:	Fc1c(Cl)c(F)c(Cl)c(F)c1Cl
Mol. weight [g/mol]:	235.42
CAS:	319-88-0

Physical Properties

Property code	Value	Unit	Source
af	0.4260		KDB
gf	-556.32	kJ/mol	Joback Method
hf	-623.54	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	53.80	kJ/mol	NIST Webbook
ie	9.48 ± 0.02	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-4.52		Crippen Method
logp	4.064		Crippen Method
mcvol	113.670	ml/mol	McGowan Method
pc	3270.00 ± 40.00	kPa	NIST Webbook
pc	3270.00	kPa	KDB
ss	243.30	J/mol×K	NIST Webbook
ss	245.35	J/mol×K	NIST Webbook
tb	471.52	K	KDB
tc	684.80	K	KDB
tc	684.80 ± 0.40	K	NIST Webbook
tf	337.93	K	Joback Method
tt	334.16 ± 0.02	K	NIST Webbook
tt	335.01 ± 0.02	K	NIST Webbook
vc	0.448	m3/kmol	KDB
zc	0.2572910		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.69	J/mol×K	532.84	Joback Method
cpg	191.70	J/mol×K	498.36	Joback Method
cpg	218.08	J/mol×K	705.24	Joback Method
cpg	214.27	J/mol×K	670.76	Joback Method
cpg	210.24	J/mol×K	636.28	Joback Method
cpg	205.96	J/mol×K	601.80	Joback Method
cpg	201.45	J/mol×K	567.32	Joback Method
cps	197.00	J/mol×K	298.15	NIST Webbook
cps	197.95	J/mol×K	298.15	NIST Webbook
hfust	19.83	kJ/mol	335.01	NIST Webbook
hfust	19.83	kJ/mol	335.00	NIST Webbook
hfust	19.83	kJ/mol	335.00	NIST Webbook
hfust	19.85	kJ/mol	334.16	NIST Webbook
hvapt	49.20	kJ/mol	430.00	NIST Webbook
sfust	59.19	J/mol×K	335.01	NIST Webbook
sfust	59.40	J/mol×K	334.16	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.70	K	1.60	NIST Webbook
tbrp	352.60	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45732e+01
Coeff. B	-4.03336e+03
Coeff. C	-6.63860e+01
Temperature range (K), min.	348.72

Temperature range (K), max.	501.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.25168e+01
Coeff. B	-9.57434e+03
Coeff. C	-1.11720e+01
Coeff. D	5.31858e-06
Temperature range (K), min.	364.00
Temperature range (K), max.	678.58

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C319880&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1663
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1663.mol

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility