Benzene, 1-chloro-2-(trifluoromethyl)-

Other names:	1-Chloro-2-(trifluoromethyl)benzene 2-(Trifluoromethyl)chlorobenzene 2-Chloro(trifluoromethyl)benzene 2-Chloro-benzotrifluoride 2-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene 2-Chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene NSC 10307 Toluene, o-chloro-«alpha»,«alpha»,«alpha»-trifluoro- Toluene, o-chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro- o-(Trifluoromethyl)chlorobenzene o-(Trifluoromethyl)phenyl chloride o-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene o-Chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene o-Chlorobenzotrifluoride
Inchi:	InChI=1S/C7H4ClF3/c8-6-4-2-1-3-5(6)7(9,10)11/h1-4H
InchiKey:	DGRVQOKCSKDWIH-UHFFFAOYSA-N
Formula:	C7H4ClF3
SMILES:	FC(F)(F)c1ccccc1Cl
Mol. weight [g/mol]:	180.56
CAS:	88-16-4

Physical Properties

Property code	Value	Unit	Source
gf	-482.68	kJ/mol	Joback Method
hf	-575.57	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
ie	9.47	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	3.359		Crippen Method
mcvol	103.280	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	883.40		NIST Webbook
rinpol	883.40		NIST Webbook
rinpol	883.40		NIST Webbook
tb	425.40	K	NIST Webbook
tc	622.89	K	Joback Method

tf	241.70	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.38	J/mol×K	556.34	Joback Method
cpg	234.75	J/mol×K	589.61	Joback Method
cpg	191.34	J/mol×K	423.23	Joback Method
cpg	201.41	J/mol×K	456.51	Joback Method
cpg	210.74	J/mol×K	489.78	Joback Method
cpg	219.39	J/mol×K	523.06	Joback Method
cpg	241.55	J/mol×K	622.89	Joback Method
hfust	11.60	kJ/mol	264.00	NIST Webbook
hvapt	44.60	kJ/mol	368.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40359e+01
Coeff. B	-3.36228e+03
Coeff. C	-6.83280e+01
Temperature range (K), min.	312.89
Temperature range (K), max.	453.71

Sources

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=C88164&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume