Benzene, 1-chloro-4-(trifluoromethyl)-

Other names:	(p-Chlorophenyl)trifluoromethane
	1-(Trifluoromethyl)-4-chlorobenzene
	1-Chloro-4-(trifluoromethyl)benzene
	4-CHLOROBENZOTRIFLUORIDE
	4-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	4-Chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
	NSC 10309
	Toluene, p-chloro-«alpha»,«alpha»,«alpha»-trifluoro-
	Toluene, p-chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-
	p-(Trifluoromethyl)chlorobenzene
	p-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	p-Chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
	p-Chlorobenzotrifluoride
	p-Chlorotrifluoromethylbenzene
	p-Trifluoromethylphenyl chloride
	para-Chlorobenzotrifluoride
Inchi:	InChI=1S/C7H4ClF3/c8-6-3-1-5(2-4-6)7(9,10)11/h1-4H
InchiKey:	QULYNCCPRWKEMF-UHFFFAOYSA-N
Formula:	C7H4ClF3
SMILES:	FC(F)(F)c1ccc(Cl)cc1
Mol. weight [g/mol]:	180.56
CAS:	98-56-6

Physical Properties

Property code	Value	Unit	Source
chs	-3329.00 ± 13.00	kJ/mol	NIST Webbook
gf	-482.68	kJ/mol	Joback Method
hf	-575.57	kJ/mol	Joback Method
hfs	-323.70 ± 1.20	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	9.56	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	836.30		NIST Webbook
rinpol	836.30		NIST Webbook
ripol	1178.40		NIST Webbook
tb	410.20	K	NIST Webbook
tb	411.70	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	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	227.38	J/mol×K	556.34	Joback Method
cpg	234.75	J/mol×K	589.61	Joback Method
cpg	241.55	J/mol×K	622.89	Joback Method
hvapt	42.20	kJ/mol	357.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45020e+01
Coeff. B	-3.56577e+03
Coeff. C	-5.10770e+01
Temperature range (K), min.	301.93
Temperature range (K), max.	439.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.43724e+01

Coeff. B	-7.57771e+03
Coeff. C	-8.65972e+00
Coeff. D	4.54808e-06
Temperature range (K), min.	237.15
Temperature range (K), max.	601.00

Sources

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=1690
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/mol1690.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98566&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

Latest version available from:

https://www.chemeo.com/cid/38-059-5/Benzene-1-chloro-4-trifluoromethyl.pdf

Generated by Cheméo on 2024-10-12 08:13:48.900311257 +0000 UTC m=+3301691.537280517.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.