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

Other names: 1-Chloro-4-(trichloromethyl)benzene
4,«alpha»,«alpha»,«alpha»-Tetrachlorotoluene
4,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Tetrachlorotoluene
4-Chlorobenzotrichloride
Toluene, p,«alpha»,«alpha»,«alpha»-tetrachloro-
Toluene, p,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-tetrachloro-
Toluene, «alpha»,«alpha»,«alpha»,p-tetrachloro-
Toluene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,p-tetrachloro-
p,«alpha»,«alpha»,«alpha»-Tetrachlorotoluene
p,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Tetrachlorotoluene
p-Chlorobenzotrichloride
p-Chlorophenyltrichloromethane
p-Trichloromethylchlorobenzene
«alpha»,«alpha»,«alpha»,4-Tetrachlorotoluene
«alpha»,«alpha»,«alpha»-Trichloro-4-chlorotoluene
Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,4-Tetrachlorotoluene
Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trichloro-4-chlorotoluene

Inchi: InChI=1S/C7H4Cl4/c8-6-3-1-5(2-4-6)7(9,10)11/h1-4H

InchiKey: LVZPKYYPPLUECL-UHFFFAOYSA-N

Formula: C7H4Cl4

SMILES: Clc1ccc(C(Cl)(Cl)Cl)cc1

Mol. weight [g/mol]: 229.92

CAS: 5216-25-1

Physical Properties

Property code	Value	Unit	Source
gf	65.96	kJ/mol	Joback Method
hf	-34.46	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.167		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1367.20		NIST Webbook
rinpol	1367.20		NIST Webbook
rinpol	1361.00		NIST Webbook

tb	518.20	K	NIST Webbook
tc	792.94	K	Joback Method
tf	329.69	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.44	J/mol×K	537.71	Joback Method
cpg	242.39	J/mol×K	580.25	Joback Method
cpg	250.40	J/mol×K	622.79	Joback Method
cpg	257.55	J/mol×K	665.32	Joback Method
cpg	263.93	J/mol×K	707.86	Joback Method
cpg	269.61	J/mol×K	750.40	Joback Method
cpg	274.69	J/mol×K	792.94	Joback Method
dvisc	0.0024728	Pa×s	329.69	Joback Method
dvisc	0.0014383	Pa×s	364.36	Joback Method
dvisc	0.0009192	Pa×s	399.03	Joback Method
dvisc	0.0006310	Pa×s	433.70	Joback Method
dvisc	0.0004580	Pa×s	468.37	Joback Method
dvisc	0.0003475	Pa×s	503.04	Joback Method
dvisc	0.0002731	Pa×s	537.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38683e+01
Coeff. B	-4.00529e+03

Coeff. C	-8.51960e+01
Temperature range (K), min.	380.12
Temperature range (K), max.	553.28

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=C5216251&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
dvisc:	Dynamic viscosity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/22-778-4/Benzene-1-chloro-4-trichloromethyl.pdf

Generated by Cheméo on 2024-10-12 09:29:39.701449995 +0000 UTC m=+3306242.338419253.

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