

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.44	J/molxK	537.71	Joback Method
cpg	242.39	J/molxK	580.25	Joback Method
cpg	250.40	J/molxK	622.79	Joback Method
cpg	257.55	J/molxK	665.32	Joback Method
cpg	263.93	J/molxK	707.86	Joback Method
cpg	269.61	J/molxK	750.40	Joback Method
cpg	274.69	J/molxK	792.94	Joback Method
dvisc	0.0024728	Paxs	329.69	Joback Method
dvisc	0.0014383	Paxs	364.36	Joback Method
dvisc	0.0009192	Paxs	399.03	Joback Method
dvisc	0.0006310	Paxs	433.70	Joback Method
dvisc	0.0004580	Paxs	468.37	Joback Method
dvisc	0.0003475	Paxs	503.04	Joback Method
dvisc	0.0002731	Paxs	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	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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

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