

Benzene, 2,4-dichloro-1-(trichloromethyl)-

Other names:	Toluene, «alpha», «alpha», «alpha», 2,4-pentachloro-1,3-Dichloro-4-(trichloromethyl)benzene 2,4-Dichlorobenzotrichloride 2,4-Dichlorophenyltrichloromethane 2,4, «alpha», «alpha», «alpha»-Pentachlorotoluene «alpha», «alpha», «alpha», 2,4-Pentachlorotoluene 2,4-dichloro-1-(trichloromethyl)benzene
Inchi:	InChI=1S/C7H3Cl5/c8-4-1-2-5(6(9)3-4)7(10,11)12/h1-3H
InchiKey:	KZSNBJMYJWDVTK-UHFFFAOYSA-N
Formula:	C7H3Cl5
SMILES:	Clc1ccc(C(Cl)(Cl)Cl)c(Cl)c1
Mol. weight [g/mol]:	264.36
CAS:	13014-18-1

Physical Properties

Property code	Value	Unit	Source
gf	44.40	kJ/mol	Joback Method
hf	-61.67	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	55.41	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.820		Crippen Method
mvol	146.930	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	580.12	K	Joback Method
tc	840.49	K	Joback Method
tf	372.13	K	Joback Method
vc	0.553	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.57	J/mol×K	580.12	Joback Method
cpg	281.92	J/mol×K	797.10	Joback Method

cpg	277.18	J/molxK	753.70	Joback Method
cpg	271.86	J/molxK	710.31	Joback Method
cpg	265.87	J/molxK	666.91	Joback Method
cpg	259.14	J/molxK	623.52	Joback Method
cpg	286.15	J/molxK	840.49	Joback Method
dvisc	0.0002450	Paxs	580.12	Joback Method
dvisc	0.0003049	Paxs	545.45	Joback Method
dvisc	0.0003910	Paxs	510.79	Joback Method
dvisc	0.0005198	Paxs	476.12	Joback Method
dvisc	0.0007226	Paxs	441.46	Joback Method
dvisc	0.0010625	Paxs	406.80	Joback Method
dvisc	0.0016788	Paxs	372.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13014181&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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