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

Other names:	Toluene, «alpha»,«alpha»,«alpha»,3,4-pentachloro- «alpha»,«alpha»,«alpha»,3,4-Pentachlorotoluene 1,2-Dichloro-4-trichloromethylbenzene 3,4-Dichlorobenzotrichloride 3,4-Dichlorophenyltrichloromethane
Inchi:	InChI=1S/C7H3Cl5/c8-5-2-1-4(3-6(5)9)7(10,11)12/h1-3H
InchiKey:	ATYLRBXENHNROH-UHFFFAOYSA-N
Formula:	C7H3Cl5
SMILES:	Clc1ccc(C(Cl)(Cl)Cl)cc1Cl
Mol. weight [g/mol]:	264.36
CAS:	13014-24-9

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
mcvol	146.930	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1534.20		NIST Webbook
rinpol	1534.20		NIST Webbook
tb	556.30	K	NIST Webbook
tc	840.49	K	Joback Method
tf	372.13	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.15	J/mol×K	840.49	Joback Method
cpg	251.57	J/mol×K	580.12	Joback Method

cpg	259.14	J/mol×K	623.52	Joback Method
cpg	265.87	J/mol×K	666.91	Joback Method
cpg	271.86	J/mol×K	710.31	Joback Method
cpg	277.18	J/mol×K	753.70	Joback Method
cpg	281.92	J/mol×K	797.10	Joback Method
dvisc	0.0002450	Pa×s	580.12	Joback Method
dvisc	0.0016788	Pa×s	372.13	Joback Method
dvisc	0.0010625	Pa×s	406.80	Joback Method
dvisc	0.0007226	Pa×s	441.46	Joback Method
dvisc	0.0005198	Pa×s	476.12	Joback Method
dvisc	0.0003910	Pa×s	510.79	Joback Method
dvisc	0.0003049	Pa×s	545.45	Joback Method
hvapt	59.30	kJ/mol	550.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13014249&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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