

2,4,5-trichlorotoluene

Other names:	Benzene, 1,2,4-trichloro-5-methyl- Benzene, 1-methyl-2,4,5-trichloro- Toluene, 2,4,5-trichloro-
Inchi:	InChI=1S/C7H5Cl3/c1-4-2-6(9)7(10)3-5(4)8/h2-3H,1H3
InchiKey:	ZCXHZKNWIYVQNC-UHFFFAOYSA-N
Formula:	C7H5Cl3
SMILES:	Cc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	195.48

Physical Properties

Property code	Value	Unit	Source
hf	-31.32	kJ/mol	Cheméo Relay (1.0)
hfus	19.35	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	NIST Webbook
log10ws	-4.82		Cheméo Relay (1.0)
logp	3.955		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
tb	504.62	K	Cheméo Relay (1.0)
tf	319.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.21	J/mol×K	513.47	Joback Method
cpg	249.42	J/mol×K	749.79	Joback Method
cpg	243.55	J/mol×K	710.40	Joback Method
cpg	237.23	J/mol×K	671.02	Joback Method
cpg	230.46	J/mol×K	631.63	Joback Method
cpg	223.21	J/mol×K	592.24	Joback Method
cpg	215.47	J/mol×K	552.86	Joback Method
dvisc	0.0005096	Pa×s	417.93	Joback Method
dvisc	0.0002778	Pa×s	513.47	Joback Method
dvisc	0.0003311	Pa×s	481.62	Joback Method

dvisc	0.0004045	Pa×s	449.78	Joback Method
dvisc	0.0013398	Pa×s	322.39	Joback Method
dvisc	0.0006669	Pa×s	386.08	Joback Method
dvisc	0.0009161	Pa×s	354.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.70	K	95.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6639301&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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