2,3,4,5,6-PENTACHLOROTOLUENE

Other names: Methylpentachlorobenzene
Toluene, 2,3,4,5,6-pentachloro-
Inchi: InChI=1S/C7H3Cl5/c1-2-3(8)5(10)7(12)6(11)4(2)9/h1H3
InchiKey: AVSIMRGRHWKCAY-UHFFFAOYSA-N
Formula: C7H3Cl5
SMILES: Cc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 264.37
CAS: 877-11-2

Physical Properties

Property code	Value	Unit	Source
af	0.4671		Cheméo Relay (1.0)
hf	-47.99	kJ/mol	Cheméo Relay (1.0)
hfus	26.97	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-6.60		Cheméo Relay (1.0)
logp	5.262		Crippen Method
mcvol	146.930	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
tb	574.90	K	Cheméo Relay (1.0)
tc	818.67	K	Cheméo Relay (1.0)
tf	497.00 ± 2.00	K	NIST Webbook
vc	0.548	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.26	J/mol×K	598.29	Joback Method
cpg	248.65	J/mol×K	639.45	Joback Method
cpg	254.64	J/mol×K	680.60	Joback Method
cpg	260.23	J/mol×K	721.76	Joback Method
cpg	265.42	J/mol×K	762.92	Joback Method
cpg	270.23	J/mol×K	804.08	Joback Method

cpg	274.67	J/mol×K	845.23	Joback Method
dvisc	0.0009073	Pa×s	407.27	Joback Method
dvisc	0.0006820	Pa×s	439.11	Joback Method
dvisc	0.0005329	Pa×s	470.94	Joback Method
dvisc	0.0004295	Pa×s	502.78	Joback Method
dvisc	0.0003552	Pa×s	534.62	Joback Method
dvisc	0.0003001	Pa×s	566.45	Joback Method
dvisc	0.0002582	Pa×s	598.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65505e+01
Coeff. B	-5.54934e+03
Coeff. C	-1.00764e+02
Temperature range (K), min.	441.99
Temperature range (K), max.	594.52

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C877112&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume