2,5-DICHLOROTOLUENE

Other names: Toluene, 2,5-dichloro-
Inchi: InChI=1S/C7H6Cl2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
InchiKey: KFAKZJUYBOYVKA-UHFFFAOYSA-N
Formula: C7H6Cl2
SMILES: Cc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 161.03
CAS: 19398-61-9

Physical Properties

Property code	Value	Unit	Source
hf	-11.00	kJ/mol	Cheméo Relay (1.0)
hfus	15.54	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Cheméo Relay (1.0)
ie	8.75 ± 0.02	eV	NIST Webbook
ie	8.81	eV	NIST Webbook
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.302		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
rinpol	1100.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	471.70	K	NIST Webbook
tc	700.61	K	Cheméo Relay (1.0)
tf	279.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.67	J/mol×K	471.06	Joback Method
cpg	195.96	J/mol×K	509.30	Joback Method
cpg	204.68	J/mol×K	547.53	Joback Method

cpg	212.85	J/mol×K	585.77	Joback Method
cpg	220.49	J/mol×K	624.01	Joback Method
cpg	227.64	J/mol×K	662.24	Joback Method
cpg	234.30	J/mol×K	700.48	Joback Method
dvisc	0.0016666	Pa×s	279.95	Joback Method
dvisc	0.0010588	Pa×s	311.80	Joback Method
dvisc	0.0007317	Pa×s	343.65	Joback Method
dvisc	0.0005384	Pa×s	375.50	Joback Method
dvisc	0.0004156	Pa×s	407.36	Joback Method
dvisc	0.0003331	Pa×s	439.21	Joback Method
dvisc	0.0002751	Pa×s	471.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40370e+01
Coeff. B	-3.75818e+03
Coeff. C	-7.26860e+01
Temperature range (K), min.	346.02
Temperature range (K), max.	503.40

Sources

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=C19398619&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point