1,2,4,5-tetrachloro-3-methylbenzene

Inchi: InChI=1S/C7H4Cl4/c1-3-6(10)4(8)2-5(9)7(3)11/h2H,1H3
InchiKey: ZOXPZFFPPKVNEA-UHFFFAOYSA-N
Formula: C7H4Cl4
SMILES: Cc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 229.92
CAS: 1006-31-1

Physical Properties

Property code	Value	Unit	Source
hf	-44.62	kJ/mol	Cheméo Relay (1.0)
hfus	23.16	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
log10ws	-5.52		Cheméo Relay (1.0)
logp	4.609		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
tb	539.25	K	Cheméo Relay (1.0)
tf	380.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.66	J/mol×K	555.88	Joback Method
cpg	232.95	J/mol×K	596.23	Joback Method
cpg	239.78	J/mol×K	636.58	Joback Method
cpg	246.17	J/mol×K	676.93	Joback Method
cpg	252.12	J/mol×K	717.28	Joback Method
cpg	257.66	J/mol×K	757.63	Joback Method
cpg	262.79	J/mol×K	797.98	Joback Method
dvisc	0.0010964	Pa×s	364.83	Joback Method
dvisc	0.0007911	Pa×s	396.67	Joback Method
dvisc	0.0005992	Pa×s	428.51	Joback Method
dvisc	0.0004716	Pa×s	460.36	Joback Method
dvisc	0.0003829	Pa×s	492.20	Joback Method

dvisc	0.0003188	Pa×s	524.04	Joback Method
dvisc	0.0002711	Pa×s	555.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45082e+01
Coeff. B	-4.32441e+03
Coeff. C	-8.98660e+01
Temperature range (K), min.	393.96
Temperature range (K), max.	560.08

Sources

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):

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

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point