1,2,5-trichloro-3-methylbenzene

Inchi: InChI=1S/C7H5Cl3/c1-4-2-5(8)3-6(9)7(4)10/h2-3H,1H3
InchiKey: OKLGPXYADUOPGA-UHFFFAOYSA-N
Formula: C7H5Cl3
SMILES: Cc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 195.48
CAS: 56961-86-5

Physical Properties

Property code	Value	Unit	Source
hf	-22.91	kJ/mol	Cheméo Relay (1.0)
hfus	19.35	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-4.71		Cheméo Relay (1.0)
logp	3.955		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
tb	508.22	K	Cheméo Relay (1.0)
tf	302.73	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	215.47	J/mol×K	552.86	Joback Method
cpg	223.21	J/mol×K	592.24	Joback Method
cpg	230.46	J/mol×K	631.63	Joback Method
cpg	237.23	J/mol×K	671.02	Joback Method
cpg	243.55	J/mol×K	710.40	Joback Method
cpg	249.42	J/mol×K	749.79	Joback Method
dvisc	0.0013398	Pa×s	322.39	Joback Method
dvisc	0.0009161	Pa×s	354.24	Joback Method
dvisc	0.0006669	Pa×s	386.08	Joback Method
dvisc	0.0005096	Pa×s	417.93	Joback Method
dvisc	0.0004045	Pa×s	449.78	Joback Method

dvisc	0.0003311	Pa×s	481.62	Joback Method
dvisc	0.0002778	Pa×s	513.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37396e+01
Coeff. B	-3.85391e+03
Coeff. C	-8.10260e+01
Temperature range (K), min.	367.52
Temperature range (K), max.	538.30

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point