1,2,3-trichloro-4-(dichloromethyl)benzene

Inchi: InChI=1S/C7H3Cl5/c8-4-2-1-3(7(11)12)5(9)6(4)10/h1-2,7H
InchiKey: GTQJFLXWDUNQKB-UHFFFAOYSA-N
Formula: C7H3Cl5
SMILES: Clc1ccc(C(Cl)Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 264.37
CAS: 56961-82-1

Physical Properties

Property code	Value	Unit	Source
hf	-68.33	kJ/mol	Cheméo Relay (1.0)
hfus	24.22	kJ/mol	Joback Method
hvap	75.33	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-4.99		Cheméo Relay (1.0)
logp	5.123		Crippen Method
mcvol	146.930	ml/mol	McGowan Method
tb	564.77	K	Cheméo Relay (1.0)
tf	348.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.28	J/mol×K	587.89	Joback Method
cpg	280.93	J/mol×K	838.40	Joback Method
cpg	276.40	J/mol×K	796.65	Joback Method
cpg	271.41	J/mol×K	754.90	Joback Method
cpg	265.93	J/mol×K	713.14	Joback Method
cpg	259.94	J/mol×K	671.39	Joback Method
cpg	253.40	J/mol×K	629.64	Joback Method
dvisc	0.0004942	Pa×s	477.56	Joback Method
dvisc	0.0002491	Pa×s	587.89	Joback Method
dvisc	0.0003036	Pa×s	551.11	Joback Method
dvisc	0.0003807	Pa×s	514.34	Joback Method
dvisc	0.0014801	Pa×s	367.23	Joback Method

dvisc	0.0006702	Pa×s	440.78	Joback Method
dvisc	0.0009607	Pa×s	404.01	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41664e+01
Coeff. B	-4.50160e+03
Coeff. C	-9.43700e+01
Temperature range (K), min.	418.72
Temperature range (K), max.	602.74

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):

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

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