1,2,4-trichloro-5-(chloromethyl)benzene

Inchi: InChI=1S/C7H4Cl4/c8-3-4-1-6(10)7(11)2-5(4)9/h1-2H,3H2
InchiKey: UBJKMVAYDQUJSJ-UHFFFAOYSA-N
Formula: C7H4Cl4
SMILES: ClCc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 229.92
CAS: 3955-26-8

Physical Properties

Property code	Value	Unit	Source
hf	-55.55	kJ/mol	Cheméo Relay (1.0)
hfus	23.55	kJ/mol	Joback Method
hvap	70.07	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-4.98		Cheméo Relay (1.0)
logp	4.386		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
tb	541.86	K	Cheméo Relay (1.0)
tf	340.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.01	J/mol×K	550.90	Joback Method
cpg	234.62	J/mol×K	591.06	Joback Method
cpg	241.70	J/mol×K	631.22	Joback Method
cpg	248.27	J/mol×K	671.38	Joback Method
cpg	254.35	J/mol×K	711.54	Joback Method
cpg	259.98	J/mol×K	751.70	Joback Method
cpg	265.16	J/mol×K	791.86	Joback Method
dvisc	0.0013337	Pa×s	352.31	Joback Method
dvisc	0.0009175	Pa×s	385.41	Joback Method
dvisc	0.0006697	Pa×s	418.51	Joback Method
dvisc	0.0005119	Pa×s	451.61	Joback Method
dvisc	0.0004059	Pa×s	484.70	Joback Method

dvisc	0.0003315	Pa×s	517.80	Joback Method
dvisc	0.0002775	Pa×s	550.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53770e+01
Coeff. B	-4.67077e+03
Coeff. C	-9.29800e+01
Temperature range (K), min.	402.52
Temperature range (K), max.	557.02

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