1,2-dichloro-4-(dichloromethyl)benzene

Inchi: InChI=1S/C7H4Cl4/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3,7H
InchiKey: LLPBAWYATBAOQG-UHFFFAOYSA-N
Formula: C7H4Cl4
SMILES: Clc1ccc(C(Cl)Cl)cc1Cl
Mol. weight [g/mol]: 229.92
CAS: 56961-84-3

Physical Properties

Property code	Value	Unit	Source
hf	-49.09	kJ/mol	Cheméo Relay (1.0)
hfus	20.41	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-4.38		Cheméo Relay (1.0)
logp	4.470		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
tb	525.60	K	Cheméo Relay (1.0)
tf	312.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.70	J/mol×K	545.48	Joback Method
cpg	236.90	J/mol×K	586.39	Joback Method
cpg	244.46	J/mol×K	627.31	Joback Method
cpg	251.40	J/mol×K	668.22	Joback Method
cpg	257.78	J/mol×K	709.13	Joback Method
cpg	263.61	J/mol×K	750.05	Joback Method
cpg	268.93	J/mol×K	790.96	Joback Method
dvisc	0.0020204	Pa×s	324.79	Joback Method
dvisc	0.0012150	Pa×s	361.57	Joback Method
dvisc	0.0008027	Pa×s	398.35	Joback Method
dvisc	0.0005687	Pa×s	435.13	Joback Method
dvisc	0.0004252	Pa×s	471.92	Joback Method

dvisc	0.0003316	Pa×s	508.70	Joback Method
dvisc	0.0002674	Pa×s	545.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41115e+01
Coeff. B	-4.16359e+03
Coeff. C	-8.85320e+01
Temperature range (K), min.	389.72
Temperature range (K), max.	561.67

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