1,1,1,2,3-pentachloropropane

Inchi: InChI=1S/C3H3Cl5/c4-1-2(5)3(6,7)8/h2H,1H2
InchiKey: ZXPCCXXSNUIVNK-UHFFFAOYSA-N
Formula: C3H3Cl5
SMILES: ClCC(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 216.32
CAS: 21700-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-84.87	kJ/mol	Joback Method
hf	-184.33	kJ/mol	Cheméo Relay (1.0)
hfus	13.57	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Cheméo Relay (1.0)
ie	10.97	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	3.203		Crippen Method
mcvol	114.330	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	465.45	K	Cheméo Relay (1.0)
tc	682.89	K	Cheméo Relay (1.0)
tf	241.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.76	J/mol×K	451.52	Joback Method
cpg	177.65	J/mol×K	489.22	Joback Method
cpg	182.95	J/mol×K	526.91	Joback Method
cpg	187.69	J/mol×K	564.61	Joback Method
cpg	191.94	J/mol×K	602.30	Joback Method
cpg	195.72	J/mol×K	640.00	Joback Method
cpg	199.09	J/mol×K	677.69	Joback Method
dvisc	0.0069460	Pa×s	260.59	Joback Method
dvisc	0.0033757	Pa×s	292.41	Joback Method

dvisc	0.0018901	Pa×s	324.23	Joback Method
dvisc	0.0011739	Pa×s	356.06	Joback Method
dvisc	0.0007884	Pa×s	387.88	Joback Method
dvisc	0.0005624	Pa×s	419.70	Joback Method
dvisc	0.0004208	Pa×s	451.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32531e+01
Coeff. B	-3.42462e+03
Coeff. C	-6.69870e+01
Temperature range (K), min.	331.12
Temperature range (K), max.	498.21

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
gf: Standard Gibbs free energy of formation
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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point