1,2,3,4-tetrachlorobutane

Inchi: InChI=1S/C4H6Cl4/c5-1-3(7)4(8)2-6/h3-4H,1-2H2
InchiKey: IXZVKECRTHXEEW-UHFFFAOYSA-N
Formula: C4H6Cl4
SMILES: ClCC(Cl)C(Cl)CCl
Mol. weight [g/mol]: 195.90
CAS: 3405-32-1

Physical Properties

Property code	Value	Unit	Source
af	0.3643		Cheméo Relay (1.0)
gf	-69.80	kJ/mol	Joback Method
hf	-228.50	kJ/mol	Cheméo Relay (1.0)
hfus	15.86	kJ/mol	Joback Method
hvap	57.96	kJ/mol	Cheméo Relay (1.0)
ie	10.50	eV	Cheméo Relay (1.0)
log10ws	-3.00		Cheméo Relay (1.0)
logp	2.679		Crippen Method
mcvol	116.180	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	471.47	K	Cheméo Relay (1.0)
tc	701.96	K	Cheméo Relay (1.0)
tf	322.50	K	Cheméo Relay (1.0)
vc	0.406	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.96	J/mol×K	439.76	Joback Method
cpg	192.20	J/mol×K	474.25	Joback Method
cpg	199.02	J/mol×K	508.75	Joback Method
cpg	205.42	J/mol×K	543.24	Joback Method
cpg	211.43	J/mol×K	577.74	Joback Method
cpg	217.06	J/mol×K	612.23	Joback Method
cpg	222.34	J/mol×K	646.72	Joback Method

dvisc	0.0086080	Pa×s	224.52	Joback Method
dvisc	0.0035403	Pa×s	260.39	Joback Method
dvisc	0.0018056	Pa×s	296.27	Joback Method
dvisc	0.0010650	Pa×s	332.14	Joback Method
dvisc	0.0006963	Pa×s	368.01	Joback Method
dvisc	0.0004909	Pa×s	403.89	Joback Method
dvisc	0.0003664	Pa×s	439.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39423e+01
Coeff. B	-3.70313e+03
Coeff. C	-6.70210e+01
Temperature range (K), min.	338.22
Temperature range (K), max.	496.08

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

af: Acentric Factor
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
vc:	Critical Volume