Chloroacetic anhydride

Inchi: InChI=1S/C4H4Cl2O3/c5-1-3(7)9-4(8)2-6/h1-2H2
InchiKey: PNVPNXKRAUBJGW-UHFFFAOYSA-N
Formula: C4H4Cl2O3
SMILES: O=C(CCl)OC(=O)CCl
Mol. weight [g/mol]: 170.98
CAS: 541-88-8

Physical Properties

Property code	Value	Unit	Source
hf	-650.19	kJ/mol	Cheméo Relay (1.0)
hfus	18.90	kJ/mol	Joback Method
hvap	46.06	kJ/mol	Cheméo Relay (1.0)
ie	10.76	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	0.534		Crippen Method
mcvol	100.710	ml/mol	McGowan Method
tb	476.68	K	Cheméo Relay (1.0)
tf	325.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.77	J/mol×K	495.94	Joback Method
cpg	185.76	J/mol×K	530.14	Joback Method
cpg	191.48	J/mol×K	564.35	Joback Method
cpg	196.92	J/mol×K	598.55	Joback Method
cpg	202.09	J/mol×K	632.75	Joback Method
cpg	206.97	J/mol×K	666.96	Joback Method
cpg	211.57	J/mol×K	701.16	Joback Method
dvisc	0.0025238	Pa×s	316.77	Joback Method
dvisc	0.0016139	Pa×s	346.63	Joback Method
dvisc	0.0011078	Pa×s	376.49	Joback Method
dvisc	0.0008037	Pa×s	406.36	Joback Method
dvisc	0.0006093	Pa×s	436.22	Joback Method

dvisc	0.0004786	Pa×s	466.08	Joback Method
dvisc	0.0003870	Pa×s	495.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64201e+01
Coeff. B	-6.22801e+03
Coeff. C	1.25000e+01
Temperature range (K), min.	340.00
Temperature range (K), max.	548.15

Sources

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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