Acetic acid, chloro-, anhydride

Other names:	Chloracetic anhydride
	Chloroacetic acid anhydride
	Chloroacetic anhydride
	Chloroacetyl anhydride
	Monochloroacetic acid anhydride
	2-Chloroacetic anhydride
	Monochloroacetic 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
gf	-403.90	kJ/mol	Joback Method
hf	-514.75	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.534		Crippen Method
mcvol	100.710	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
tb	476.20	K	NIST Webbook
tc	701.16	K	Joback Method
tf	316.77	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	211.57	J/mol×K	701.16	Joback Method
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
dvisc	0.0003870	Pa×s	495.94	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
hvapt	61.80	kJ/mol	415.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	2.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C541888&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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