

Acetic acid, chloro-, anhydride

Other names:	Chloroacetic 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
mvol	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
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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	Paxs	316.77	Joback Method
dvisc	0.0016139	Paxs	346.63	Joback Method
dvisc	0.0011078	Paxs	376.49	Joback Method
dvisc	0.0008037	Paxs	406.36	Joback Method
dvisc	0.0006093	Paxs	436.22	Joback Method
dvisc	0.0004786	Paxs	466.08	Joback Method
dvisc	0.0003870	Paxs	495.94	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

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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