

Acetic acid, trichloro-, anhydride

Other names:	Trichloroacetic anhydride
Inchi:	InChI=1S/C4Cl6O3/c5-3(6,7)1(11)13-2(12)4(8,9)10
InchiKey:	MEFKFJOEVLUFAY-UHFFFAOYSA-N
Formula:	C4Cl6O3
SMILES:	O=C(OC(=O)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	308.76
CAS:	4124-31-6

Physical Properties

Property code	Value	Unit	Source
gf	-445.94	kJ/mol	Joback Method
hf	-595.21	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	64.12	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.797		Crippen Method
mcvol	149.670	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1471.00		NIST Webbook
tb	639.20	K	Joback Method
tc	889.45	K	Joback Method
tf	441.29	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.09	J/molxK	639.20	Joback Method
cpg	260.96	J/molxK	680.91	Joback Method
cpg	264.20	J/molxK	722.62	Joback Method
cpg	266.87	J/molxK	764.32	Joback Method
cpg	269.06	J/molxK	806.03	Joback Method
cpg	270.82	J/molxK	847.74	Joback Method
cpg	272.23	J/molxK	889.45	Joback Method

dvisc	0.0015703	Paxs	441.29	Joback Method
dvisc	0.0010083	Paxs	474.28	Joback Method
dvisc	0.0006859	Paxs	507.26	Joback Method
dvisc	0.0004890	Paxs	540.25	Joback Method
dvisc	0.0003625	Paxs	573.23	Joback Method
dvisc	0.0002776	Paxs	606.22	Joback Method
dvisc	0.0002186	Paxs	639.20	Joback Method
hvapt	56.00	kJ/mol	412.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	8.00	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=C4124316&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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