Trichloroacetic Acid

Other names:	Acetic acid, trichloro-
	Aceto-Caustin
	Amchem Grass Killer
	Trichloroethanoic acid
	TCA
	CCl3COOH
	Acide trichloracetique
	Acido tricloroacetico
	Trichloorazijnzuur
	Trichloracetic acid
	Trichloressigsaeure
	Konesta
	Kyselina trichloroctova
	UN 1839
	TKhUK
	TKhU
	Acetic acid, 2,2,2-trichloro-
	NSC 215204
Inchi:	InChI=1S/C2HCl3O2/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey:	YNJBWRMUSHSURL-UHFFFAOYSA-N
Formula:	C2HCl3O2
SMILES:	O=C(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	163.39
CAS:	76-03-9

Physical Properties

Property code	Value	Unit	Source
affp	770.00	kJ/mol	NIST Webbook
basg	739.10	kJ/mol	NIST Webbook
chs	-497.50 ± 8.40	kJ/mol	NIST Webbook
chs	-490.80	kJ/mol	NIST Webbook
gf	-332.73	kJ/mol	Joback Method
hf	-433.67	kJ/mol	NIST Webbook
hfus	11.80	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.441		Crippen Method

mcvol	83.200	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
rinpol	1390.00		NIST Webbook
tb	470.70	K	NIST Webbook
tb	469.20	K	NIST Webbook
tb	468.35 ± 0.50	K	NIST Webbook
tc	708.15	K	Joback Method
tf	332.25 ± 0.10	K	NIST Webbook
tf	332.00 ± 1.50	K	NIST Webbook
tf	332.31 ± 0.07	K	NIST Webbook
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.69	J/mol×K	673.50	Joback Method
cpg	143.67	J/mol×K	638.85	Joback Method
cpg	147.47	J/mol×K	708.15	Joback Method
cpg	132.55	J/mol×K	500.27	Joback Method
cpg	135.84	J/mol×K	534.92	Joback Method
cpg	138.78	J/mol×K	569.56	Joback Method
cpg	141.38	J/mol×K	604.21	Joback Method
cps	314.00	J/mol×K	304.50	NIST Webbook
dvisc	0.0006699	Pa×s	438.59	Joback Method
dvisc	0.0004136	Pa×s	469.43	Joback Method
dvisc	0.0002710	Pa×s	500.27	Joback Method
dvisc	0.0118413	Pa×s	315.23	Joback Method
dvisc	0.0047663	Pa×s	346.07	Joback Method
dvisc	0.0022266	Pa×s	376.91	Joback Method
dvisc	0.0011671	Pa×s	407.75	Joback Method
hfust	5.90	kJ/mol	332.25	NIST Webbook
hfust	5.88	kJ/mol	330.70	NIST Webbook
hfust	5.88	kJ/mol	330.70	NIST Webbook
hvapt	57.20	kJ/mol	427.50	NIST Webbook
hvapt	65.00	kJ/mol	399.50	NIST Webbook
sfust	17.75	J/mol×K	332.25	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.70	K	3.30	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=C76039&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hfust: Enthalpy of fusion at a given temperature
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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume