Trifluoroacetic acid

Other names:	Acetic acid, 2,2,2-trifluoro- CF3COOH Kyselina trifluoroctova NSC 77366 Perfluoroacetic acid Trifluoracetic acid UN 2699 acetic acid, trifluoro- trifluoroethanoic acid
Inchi:	InChI=1S/C2HF3O2/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey:	DTQVDTLACAAQTR-UHFFFAOYSA-N
Formula:	C2HF3O2
SMILES:	O=C(O)C(F)(F)F
Mol. weight [g/mol]:	114.02
CAS:	76-05-1

Physical Properties

Property code	Value	Unit	Source
affp	711.70	kJ/mol	NIST Webbook
basg	680.70	kJ/mol	NIST Webbook
chl	-397.20 ± 1.50	kJ/mol	NIST Webbook
gf	-881.37	kJ/mol	Joback Method
hf	-1031.40 ± 1.70	kJ/mol	NIST Webbook
hf	-1018.00 ± 4.60	kJ/mol	NIST Webbook
hfl	-1069.90 ± 1.50	kJ/mol	NIST Webbook
hfus	8.45	kJ/mol	Joback Method
hvap	41.00 ± 3.00	kJ/mol	NIST Webbook
ie	11.46	eV	NIST Webbook
ie	11.50	eV	NIST Webbook
ie	12.06	eV	NIST Webbook
ie	12.08 ± 0.05	eV	NIST Webbook
ie	12.00	eV	NIST Webbook
ie	11.60	eV	NIST Webbook
ie	12.00 ± 0.03	eV	NIST Webbook
ie	12.00	eV	NIST Webbook
log10ws	-0.42		Crippen Method
logp	0.633		Crippen Method

mcvol	51.790	ml/mol	McGowan Method
pc	5320.16	kPa	Joback Method
rinpol	744.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	744.00		NIST Webbook
tb	345.70 ± 1.00	K	NIST Webbook
tb	345.60	K	NIST Webbook
tb	345.10 ± 0.20	K	NIST Webbook
tb	347.00	K	NIST Webbook
tb	344.91	K	Isobaric vapor-liquid equilibrium of trifluoroacetic acid + water, trifluoroacetic acid + ethyl trifluoroacetate and ethyl trifluoroacetate + ethanol binary mixtures
tb	347.00	K	NIST Webbook
tc	545.18	K	Joback Method
tf	288.43 ± 0.20	K	NIST Webbook
tf	531.17 ± 0.20	K	NIST Webbook
vc	0.215	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.53	J/mol×K	518.61	Joback Method
cpg	105.37	J/mol×K	385.79	Joback Method
cpg	109.52	J/mol×K	412.35	Joback Method
cpg	113.39	J/mol×K	438.92	Joback Method
cpg	117.02	J/mol×K	465.48	Joback Method
cpg	120.39	J/mol×K	492.05	Joback Method
cpg	126.44	J/mol×K	545.18	Joback Method
hvapt	35.90	kJ/mol	315.00	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=C76051&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Isobaric vapor-liquid equilibrium of trifluoroacetic acid + water, trifluoroacetic acid + ethyl trifluoroacetate and ethyl trifluoroacetate + ethanol binary mixtures https://www.doi.org/10.1016/j.fluid.2015.08.012

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume