Fluoroacetic acid

Other names:	2-Fluoroacetic acid
	Acetic acid, 2-fluoro-
	Acetic acid, fluoro-
	Acide-monofluoracetique
	Acido monofluoroacetio
	CH2FCOOH
	CYMONIC ACID
	Fluoroethanoic acid
	Gifblaar poison
	HFA
	MONOFLUOROACETIC ACID
	Monofluorazijnzuur
	Monofluoressigsaure
	UN 2642
Inchi:	InChI=1S/C2H3FO2/c3-1-2(4)5/h1H2,(H,4,5)
InchiKey:	QEWYKACRFQMRMB-UHFFFAOYSA-N
Formula:	C2H3FO2
SMILES:	O=C(O)CF
Mol. weight [g/mol]:	78.04
CAS:	144-49-0

Physical Properties

Property code	Value	Unit	Source
affp	765.40	kJ/mol	NIST Webbook
basg	734.50	kJ/mol	NIST Webbook
chl	-714.84	kJ/mol	NIST Webbook
gf	-494.59	kJ/mol	Joback Method
hf	-545.53	kJ/mol	Joback Method
hfus	9.70	kJ/mol	Joback Method
hvap	42.65	kJ/mol	Joback Method
log10ws	0.39		Crippen Method
logp	0.040		Crippen Method
mcvol	48.250	ml/mol	McGowan Method
pc	5917.16	kPa	Joback Method
tb	390.48	K	Joback Method
tc	557.09	K	Joback Method
tf	308.45	K	KDB

vc	0.191	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.32	J/mol×K	390.48	Joback Method
cpg	89.91	J/mol×K	418.25	Joback Method
cpg	93.37	J/mol×K	446.02	Joback Method
cpg	96.69	J/mol×K	473.78	Joback Method
cpg	99.88	J/mol×K	501.55	Joback Method
cpg	102.94	J/mol×K	529.32	Joback Method
cpg	105.87	J/mol×K	557.09	Joback Method
hvapt	52.30	kJ/mol	368.00	NIST Webbook
hvapt	53.60	kJ/mol	368.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.91428e+01
Coeff. B	-3.99864e+03
Coeff. C	7.15500e+00
Coeff. D	-3.71975e-06
Temperature range (K), min.	323.15
Temperature range (K), max.	443.15

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1781

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C144490&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1781

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

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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume