Methyl fluoroacetate

Other names:	Acetic acid, fluoro-, methyl ester
	Fluoracetic acid methyl ester
	Fluoroacetic acid, methyl ester
	MFA
	Methylester kyseliny fluoroctove
	TL 551
Inchi:	InChI=1S/C3H5FO2/c1-6-3(5)2-4/h2H2,1H3
InchiKey:	RJBYSQHLLIHSLT-UHFFFAOYSA-N
Formula:	C3H5FO2
SMILES:	COC(=O)CF
Mol. weight [g/mol]:	92.07
CAS:	453-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-454.35	kJ/mol	Joback Method
hf	-546.16	kJ/mol	Joback Method
hfus	9.39	kJ/mol	Joback Method
hvap	30.61	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	0.129		Crippen Method
mcvol	62.340	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	377.70	K	NIST Webbook
tc	513.10	K	Joback Method
tf	196.32	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.67	J/mol×K	484.85	Joback Method
cpg	106.62	J/mol×K	343.60	Joback Method
cpg	111.64	J/mol×K	371.85	Joback Method

cpg	116.56	J/mol×K	400.10	Joback Method
cpg	121.38	J/mol×K	428.35	Joback Method
cpg	126.08	J/mol×K	456.60	Joback Method
cpg	135.13	J/mol×K	513.10	Joback Method
hvapt	42.70	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.81981e+01
Coeff. B	-5.12838e+03
Temperature range (K), min.	273.00
Temperature range (K), max.	397.96

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=C453189&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

Legend

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