Propane, 2-fluoro-2-methyl-

Other names:	2-Fluoro-2-methylpropane
	tert-Butyl Fluoride
Inchi:	InChI=1S/C4H9F/c1-4(2,3)5/h1-3H3
InchiKey:	GSMZLBOYBDRGBN-UHFFFAOYSA-N
Formula:	C4H9F
SMILES:	CC(C)(C)F
Mol. weight [g/mol]:	76.11
CAS:	353-61-7

Physical Properties

Property code	Value	Unit	Source
gf	-209.17	kJ/mol	Joback Method
hf	-330.75	kJ/mol	Joback Method
hfus	1.78	kJ/mol	Joback Method
hvap	22.39	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.754		Crippen Method
mcvol	68.990	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	432.00		NIST Webbook
tb	286.96	K	Joback Method
tc	449.51	K	Joback Method
tf	137.85	K	Joback Method
vc	0.267	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.57	J/mol×K	422.42	Joback Method
cpg	101.74	J/mol×K	286.96	Joback Method
cpg	110.49	J/mol×K	314.05	Joback Method
cpg	118.83	J/mol×K	341.14	Joback Method
cpg	126.78	J/mol×K	368.23	Joback Method
cpg	134.35	J/mol×K	395.33	Joback Method

cpg	148.43	J/mol×K	449.51	Joback Method
hvapt	27.60	kJ/mol	268.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35144e+01
Coeff. B	-2.27566e+03
Coeff. C	-3.28110e+01
Temperature range (K), min.	196.15
Temperature range (K), max.	310.23

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=C353617&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

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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