Hexane, 1-fluoro-

Other names:	1-Fluorohexane
	Fluorohexane
	Hexyl fluoride
	N-HEXYL FLUORIDE
Inchi:	InChI=1S/C6H13F/c1-2-3-4-5-6-7/h2-6H2,1H3
InchiKey:	OFERIJCSHDJMSA-UHFFFAOYSA-N
Formula:	C6H13F
SMILES:	CCCCCCF
Mol. weight [g/mol]:	104.17
CAS:	373-14-8

Physical Properties

Property code	Value	Unit	Source
gf	-195.17	kJ/mol	Joback Method
hf	-363.28	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	28.13	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.536		Crippen Method
mcvol	97.170	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	656.80		NIST Webbook
rinpol	656.80		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	658.00		NIST Webbook
tb	364.70	K	NIST Webbook
tb	366.52	K	KDB
tc	490.31	K	Joback Method
tf	157.97	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	166.76	J/mol×K	335.95	Joback Method
cpg	176.71	J/mol×K	361.68	Joback Method
cpg	186.35	J/mol×K	387.40	Joback Method
cpg	195.66	J/mol×K	413.13	Joback Method
cpg	204.65	J/mol×K	438.85	Joback Method
cpg	213.34	J/mol×K	464.58	Joback Method
cpg	221.73	J/mol×K	490.31	Joback Method
hvapt	36.90	kJ/mol	330.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45279e+01
Coeff. B	-3.19264e+03
Coeff. C	-4.25230e+01
Temperature range (K), min.	266.72
Temperature range (K), max.	388.93

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.96315e+01
Coeff. B	-7.21639e+03
Coeff. C	-1.12783e+01
Coeff. D	9.82988e-06
Temperature range (K), min.	273.15
Temperature range (K), max.	388.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C373148&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1635

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1635.mol

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