n-Propyl fluoride

Other names:	1-Fluoropropane
	PROPYL FLUORIDE
	Propane, 1-fluoro-
	n-C3H7F
Inchi:	InChI=1S/C3H7F/c1-2-3-4/h2-3H2,1H3
InchiKey:	JRHNUZCXXOTJCA-UHFFFAOYSA-N
Formula:	C3H7F
SMILES:	CCCF
Mol. weight [g/mol]:	62.09
CAS:	460-13-9

Physical Properties

Property code	Value	Unit	Source
af	0.2270		KDB
gf	-220.43	kJ/mol	Joback Method
hf	-301.36	kJ/mol	Joback Method
hfus	6.61	kJ/mol	Joback Method
hvap	21.46	kJ/mol	Joback Method
ie	11.30	eV	NIST Webbook
ie	11.96	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.366		Crippen Method
mcvol	54.900	ml/mol	McGowan Method
pc	4160.00	kPa	KDB
rinpol	389.00		NIST Webbook
rinpol	389.00		NIST Webbook
tb	270.00	K	KDB
tb	269.95 ± 1.00	K	NIST Webbook
tc	422.00	K	KDB
tf	114.00	K	KDB
vc	0.222	m3/kmol	KDB
zc	0.2626140		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.05	J/mol×K	267.31	Joback Method
cpg	81.56	J/mol×K	292.28	Joback Method
cpg	86.90	J/mol×K	317.25	Joback Method
cpg	92.09	J/mol×K	342.22	Joback Method
cpg	97.12	J/mol×K	367.19	Joback Method
cpg	102.00	J/mol×K	392.16	Joback Method
cpg	106.73	J/mol×K	417.13	Joback Method
hvapt	24.00	kJ/mol	242.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41156e+01
Coeff. B	-2.24850e+03
Coeff. C	-3.31980e+01
Temperature range (K), min.	195.80
Temperature range (K), max.	288.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.45043e+00
Coeff. B	-3.03343e+03
Coeff. C	1.29921e+00
Coeff. D	-1.22237e-05
Temperature range (K), min.	195.15
Temperature range (K), max.	305.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1596
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/mol1596.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C460139&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
zc:	Critical Compressibility

Latest version available from:

https://www.chemeo.com/cid/58-951-2/n-Propyl-fluoride.pdf

Generated by Cheméo on 2024-10-12 09:22:16.842356145 +0000 UTC m=+3305799.479325393.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.