

1-Fluorononane

Other names:	Nonane, 1-fluoro- n-Nonyl fluoride
Inchi:	InChI=1S/C9H19F/c1-2-3-4-5-6-7-8-9-10/h2-9H2,1H3
InchiKey:	ITPAUTYYXIENLO-UHFFFAOYSA-N
Formula:	C9H19F
SMILES:	CCCCCCCCCF
Mol. weight [g/mol]:	146.25
CAS:	463-18-3

Physical Properties

Property code	Value	Unit	Source
chl	-5962.50 ± 2.00	kJ/mol	NIST Webbook
gf	-169.91	kJ/mol	Joback Method
hf	-423.50 ± 2.20	kJ/mol	NIST Webbook
hfl	-474.30 ± 2.00	kJ/mol	NIST Webbook
hfus	22.15	kJ/mol	Joback Method
hvap	50.84 ± 0.88	kJ/mol	NIST Webbook
hvap	50.80 ± 0.90	kJ/mol	NIST Webbook
log10ws	-3.44		Crippen Method
logp	3.706		Crippen Method
mcvol	139.440	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	440.70	K	NIST Webbook
tc	559.51	K	Joback Method
tf	191.78	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.83	J/mol×K	404.59	Joback Method
cpg	294.29	J/mol×K	430.41	Joback Method
cpg	307.27	J/mol×K	456.23	Joback Method
cpg	319.80	J/mol×K	482.05	Joback Method

cpg	331.88	J/mol×K	507.87	Joback Method
cpg	343.53	J/mol×K	533.69	Joback Method
cpg	354.75	J/mol×K	559.51	Joback Method
hvapt	46.80	kJ/mol	403.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44523e+01
Coeff. B	-3.71913e+03
Coeff. C	-6.29560e+01
Temperature range (K), min.	325.52
Temperature range (K), max.	469.83

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=C463183&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

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
hfl:	Liquid phase 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

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