1-Fluorooctane

Other names: Octane, 1-fluoro-
Octyl fluoride
n-Octyl fluoride
Inchi: InChI=1S/C8H17F/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3
InchiKey: DHIVLKMGKIZOHF-UHFFFAOYSA-N
Formula: C8H17F
SMILES: CCCCCCCCF
Mol. weight [g/mol]: 132.22
CAS: 463-11-6

Physical Properties

Property code	Value	Unit	Source
chl	-5318.00	kJ/mol	NIST Webbook
gf	-178.33	kJ/mol	Joback Method
hf	-404.56	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	49.68	kJ/mol	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.316		Crippen Method
mcvol	125.350	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	857.90		NIST Webbook
rinpol	859.60		NIST Webbook
tb	415.50	K	NIST Webbook
tb	415.70	K	NIST Webbook
tc	536.73	K	Joback Method
tf	180.51	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.42	J/mol×K	381.71	Joback Method
cpg	252.82	J/mol×K	407.55	Joback Method

cpg	264.79	J/mol×K	433.38	Joback Method
cpg	276.35	J/mol×K	459.22	Joback Method
cpg	287.50	J/mol×K	485.05	Joback Method
cpg	298.25	J/mol×K	510.89	Joback Method
cpg	308.62	J/mol×K	536.73	Joback Method
hvapt	44.10	kJ/mol	376.50	NIST Webbook
hvapt	40.43	kJ/mol	415.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45988e+01
Coeff. B	-3.58804e+03
Coeff. C	-5.66450e+01
Temperature range (K), min.	307.36
Temperature range (K), max.	442.98

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=C463116&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

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