Heptane, 1-fluoro-

Other names:	1-Fluoroheptane
	N-HEPTYL FLUORIDE
Inchi:	InChI=1S/C7H15F/c1-2-3-4-5-6-7-8/h2-7H2,1H3
InchiKey:	BITLXSQYFZTQGC-UHFFFAOYSA-N
Formula:	C7H15F
SMILES:	CCCCCCCF
Mol. weight [g/mol]:	118.19
CAS:	661-11-0

Physical Properties

Property code	Value	Unit	Source
chl	-4692.40	kJ/mol	NIST Webbook
gf	-186.75	kJ/mol	Joback Method
hf	-383.92	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	30.36	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.926		Crippen Method
mcvol	111.260	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	757.40		NIST Webbook
tb	391.10	K	NIST Webbook
tb	392.85	K	KDB
tc	513.69	K	Joback Method
tf	169.24	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.35	J/mol×K	358.83	Joback Method
cpg	213.59	J/mol×K	384.64	Joback Method
cpg	224.44	J/mol×K	410.45	Joback Method
cpg	234.93	J/mol×K	436.26	Joback Method

cpg	245.05	J/mol×K	462.07	Joback Method
cpg	254.82	J/mol×K	487.88	Joback Method
cpg	264.24	J/mol×K	513.69	Joback Method
hvapt	40.30	kJ/mol	355.00	NIST Webbook
hvapt	40.80	kJ/mol	352.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45943e+01
Coeff. B	-3.40469e+03
Coeff. C	-4.98620e+01
Temperature range (K), min.	287.84
Temperature range (K), max.	416.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.62822e+01
Coeff. B	-8.05082e+03
Coeff. C	-1.21485e+01
Coeff. D	9.39053e-06
Temperature range (K), min.	287.15
Temperature range (K), max.	417.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C661110&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=1640
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/mol1640.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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