Perfluoro-1-heptene

Other names:	1-Heptene, 1,1,2,3,3,4,4,5,5,6,6,7,7,7-tetradecafluoro-
	Hept-1-ene, perfluoro
	Perfluoro heptene-1
	Tetradecafluoro-1-heptene
	perfluorohept-1-ene
Inchi:	InChI=1S/C7F14/c8-1(2(9)10)3(11,12)4(13,14)5(15,16)6(17,18)7(19,20)21
InchiKey:	CDAVUOSPHHTNBU-UHFFFAOYSA-N
Formula:	C7F14
SMILES:	FC(F)=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	350.05
CAS:	355-63-5

Physical Properties

Property code	Value	Unit	Source
gf	-2641.96	kJ/mol	Joback Method
hf	-2879.46	kJ/mol	Joback Method
hfus	17.52	kJ/mol	Joback Method
hvap	13.38	kJ/mol	Joback Method
ie	10.48 ± 0.02	eV	NIST Webbook
log10ws	-5.57		Crippen Method
logp	5.168		Crippen Method
mcvol	129.970	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	312.00		NIST Webbook
tb	354.00 ± 3.00	K	NIST Webbook
tb	354.00 ± 1.00	K	NIST Webbook
tc	453.23	K	Joback Method
tf	156.01	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.90	J/mol×K	337.11	Joback Method

cpg	304.92	J/mol×K	356.46	Joback Method
cpg	316.25	J/mol×K	375.82	Joback Method
cpg	326.90	J/mol×K	395.17	Joback Method
cpg	336.90	J/mol×K	414.52	Joback Method
cpg	346.27	J/mol×K	433.87	Joback Method
cpg	355.04	J/mol×K	453.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50264e+01
Coeff. B	-3.27224e+03
Coeff. C	-3.96040e+01
Temperature range (K), min.	261.62
Temperature range (K), max.	376.43

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C355635&Units=SI

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

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

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