Perfluoronaphthalene

Other names:	Naphthalene, octafluoro-
	OCTAFLUORONAPHTHALENE
Inchi:	InChI=1S/C10F8/c11-3-1-2(5(13)9(17)7(3)15)6(14)10(18)8(16)4(1)12
InchiKey:	JDCMOHAFGDQQJX-UHFFFAOYSA-N
Formula:	C10F8
SMILES:	Fc1c(F)c(F)c2c(F)c(F)c(F)c(F)c2c1F
Mol. weight [g/mol]:	272.09
CAS:	313-72-4

Physical Properties

Property code	Value	Unit	Source
gf	-1383.14	kJ/mol	Joback Method
hf	-1482.77	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	40.53	kJ/mol	Joback Method
ie	8.87 ± 0.02	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
log10ws	-5.93		Crippen Method
logp	3.953		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	186.73		NIST Webbook
rinpol	189.20		NIST Webbook
rinpol	186.73		NIST Webbook
ripol	162.99		NIST Webbook
ripol	162.99		NIST Webbook
tb	482.00	K	KDB
tc	673.10	K	KDB
tf	360.60	K	KDB
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.92	J/mol×K	645.97	Joback Method
cpg	275.09	J/mol×K	507.86	Joback Method
cpg	281.81	J/mol×K	535.48	Joback Method
cpg	288.24	J/mol×K	563.10	Joback Method
cpg	294.40	J/mol×K	590.73	Joback Method
cpg	300.29	J/mol×K	618.35	Joback Method
cpg	311.29	J/mol×K	673.59	Joback Method
hfust	17.55	kJ/mol	358.80	NIST Webbook
hsubt	79.40 ± 2.50	kJ/mol	308.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.22011e+01
Coeff. B	-2.59380e+03
Coeff. C	-1.42084e+02
Temperature range (K), min.	359.80
Temperature range (K), max.	518.56

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C313724&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1708.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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