Pentane, dodecafluoro-

Other names:	DODECAFLUOROPENTANE
	Perfluoro-n-pentane
	Perfluoropentane
	n-Perfluoropentane
Inchi:	InChI=1S/C5F12/c6-1(7,2(8,9)4(12,13)14)3(10,11)5(15,16)17
InchiKey:	NJCBUSHGCBERSK-UHFFFAOYSA-N
Formula:	C5F12
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	288.03
CAS:	678-26-2

Physical Properties

Property code	Value	Unit	Source
af	0.4320		KDB
dm	0.00	debye	KDB
gf	-2332.30	kJ/mol	Joback Method
hf	-2543.60	kJ/mol	Joback Method
hfus	8.60	kJ/mol	Joback Method
hvap	26.60	kJ/mol	NIST Webbook
hvap	27.50	kJ/mol	NIST Webbook
log10ws	-4.18		Crippen Method
logp	4.017		Crippen Method
mcvol	102.550	ml/mol	McGowan Method
pc	2045.00	kPa	KDB
tb	303.20	K	NIST Webbook
tb	302.40	K	KDB
tb	302.60	K	NIST Webbook
tc	421.90 ± 0.50	K	NIST Webbook
tc	420.59	K	KDB
tf	263.00	K	KDB
tt	148.35 ± 0.30	K	NIST Webbook
vc	0.473	m3/kmol	KDB
zc	0.2766040		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.41	J/mol×K	364.88	Joback Method
cpg	263.40	J/mol×K	383.87	Joback Method
cpg	212.63	J/mol×K	288.89	Joback Method
cpg	224.00	J/mol×K	307.89	Joback Method
cpg	234.73	J/mol×K	326.88	Joback Method
cpg	244.87	J/mol×K	345.88	Joback Method
cpg	271.83	J/mol×K	402.87	Joback Method
cpl	188.30	J/mol×K	293.00	NIST Webbook
hfust	6.80	kJ/mol	147.80	NIST Webbook
hfust	6.80	kJ/mol	147.80	NIST Webbook
hsubt	43.70	kJ/mol	145.00	NIST Webbook
hvapt	31.10	kJ/mol	262.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52624e+01
Coeff. B	-2.95264e+03
Coeff. C	-2.52030e+01
Temperature range (K), min.	222.38
Temperature range (K), max.	321.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.00755e+01
Coeff. B	-5.44214e+03
Coeff. C	-8.44734e+00
Coeff. D	8.57661e-06
Temperature range (K), min.	282.00
Temperature range (K), max.	338.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies:	https://www.doi.org/10.1016/j.jct.2007.04.002
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C678262&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1614
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1614.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
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
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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