Cyclohexane, dodecafluoro-

Other names:	DODECAFLUOROCYCLOHEXANE
	Perfluorocyclohexane
Inchi:	InChI=1S/C6F12/c7-1(8)2(9,10)4(13,14)6(17,18)5(15,16)3(1,11)12
InchiKey:	RKIMETXDACNTIE-UHFFFAOYSA-N
Formula:	C6F12
SMILES:	FC1(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1(F)F
Mol. weight [g/mol]:	300.05
CAS:	355-68-0

Physical Properties

Property code	Value	Unit	Source
af	0.4320		KDB
chl	-1330.80 ± 7.60	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	-2385.12	kJ/mol	Joback Method
hf	-2476.43	kJ/mol	Joback Method
hfus	7.66	kJ/mol	Joback Method
hvap	36.00	kJ/mol	NIST Webbook
hvap	35.98	kJ/mol	NIST Webbook
ie	13.20	eV	NIST Webbook
log10ws	-4.11		Crippen Method
logp	3.812		Crippen Method
mcvol	105.780	ml/mol	McGowan Method
pc	2430.00	kPa	KDB
rinpol	248.00		NIST Webbook
rinpol	278.00		NIST Webbook
rinpol	278.00		NIST Webbook
tb	323.76	K	KDB
tc	457.20	K	KDB
tf	321.60	K	KDB
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.63	J/mol×K	347.53	Joback Method
cpg	254.59	J/mol×K	369.51	Joback Method
cpg	267.09	J/mol×K	391.48	Joback Method
cpg	278.23	J/mol×K	413.45	Joback Method
cpg	288.13	J/mol×K	435.42	Joback Method
cpg	225.08	J/mol×K	325.56	Joback Method
cpg	296.90	J/mol×K	457.40	Joback Method
hsubt	36.40	kJ/mol	289.00	NIST Webbook
hsubt	36.20	kJ/mol	313.00	NIST Webbook
hvapt	28.00	kJ/mol	415.00	NIST Webbook
hvapt	28.10	kJ/mol	400.50	NIST Webbook
hvapt	29.60	kJ/mol	365.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41940e+01
Coeff. B	-2.90945e+03
Coeff. C	-2.18740e+01
Temperature range (K), min.	226.95
Temperature range (K), max.	349.42

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.50618e+02
Coeff. B	-1.73517e+04
Coeff. C	-5.15264e+01
Coeff. D	5.09816e-05
Temperature range (K), min.	280.00
Temperature range (K), max.	400.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C355680&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=1626
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/mol1626.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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