Perfluoro(2-methylpentane)

Other names:	1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)pentane
	2-Perfluoromethylpentane
	PERFLUORO-2-METHYLPENTANE
	Pentane, 1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)-
	Pentane, undecafluoro-2-(trifluoromethyl)-
Inchi:	InChI=1S/C6F14/c7-1(4(12,13)14,5(15,16)17)2(8,9)3(10,11)6(18,19)20
InchiKey:	ROVMKEZVKFJNBD-UHFFFAOYSA-N
Formula:	C6F14
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	338.04
CAS:	355-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-2710.66	kJ/mol	Joback Method
hf	-2965.21	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	31.40	kJ/mol	NIST Webbook
log10ws	-4.91		Crippen Method
logp	4.652		Crippen Method
mcvol	120.180	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
tb	307.08	K	Joback Method
tc	418.08	K	Joback Method
tf	180.16	K	Joback Method
tt	102.45 ± 0.30	K	NIST Webbook
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.70	J/mol×K	307.08	Joback Method
cpg	276.21	J/mol×K	325.58	Joback Method
cpg	288.03	J/mol×K	344.08	Joback Method

cpg	299.18	J/mol×K	362.58	Joback Method
cpg	309.69	J/mol×K	381.08	Joback Method
cpg	319.57	J/mol×K	399.58	Joback Method
cpg	328.86	J/mol×K	418.08	Joback Method
hvapt	34.50	kJ/mol	291.00	NIST Webbook
hvapt	32.50	kJ/mol	309.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.77065e+02
Coeff. B	-9.52659e+03
Coeff. C	-2.54391e+01
Coeff. D	3.59459e-05
Temperature range (K), min.	253.15
Temperature range (K), max.	346.00

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
KDB: https://www.cheric.org/files/research/kdb/mol/mol1628.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C355044&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1628

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
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