Perfluorododecane

Other names: dodecane, hexacosafluoro-
hexacosafluorododecane
n-Perfluorododecane
Inchi: InChI=1S/C12F26/c13-1(14,3(17,18)5(21,22)7(25,26)9(29,30)11(33,34)35)2(15,16)4(19,2
InchiKey: WNZGTRLARPEMIG-UHFFFAOYSA-N
Formula: C12F26
SMILES: FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F
Mol. weight [g/mol]: 638.09
CAS: 307-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-4980.82	kJ/mol	Joback Method
hf	-5494.87	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons
hvap	5.51	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.464		Crippen Method
mcvol	225.960	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
rinpol	528.00		NIST Webbook
rinpol	528.00		NIST Webbook
ss	763.30	J/mol×K	NIST Webbook
tb	416.22	K	Joback Method
tc	517.74	K	Joback Method
tf	348.50 ± 0.50	K	NIST Webbook
tf	348.00 ± 0.10	K	NIST Webbook
tf	347.60 ± 0.20	K	NIST Webbook
tf	348.20 ± 0.20	K	NIST Webbook
tf	347.30 ± 0.20	K	NIST Webbook
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.98	J/mol×K	416.22	Joback Method
cpg	700.59	J/mol×K	500.82	Joback Method
cpg	688.41	J/mol×K	483.90	Joback Method
cpg	675.39	J/mol×K	466.98	Joback Method
cpg	661.50	J/mol×K	450.06	Joback Method
cpg	646.71	J/mol×K	433.14	Joback Method
cpg	711.97	J/mol×K	517.74	Joback Method
cps	546.80	J/mol×K	298.15	NIST Webbook
hfust	38.16	kJ/mol	348.50	NIST Webbook
hfust	6.90	kJ/mol	170.20	NIST Webbook
hfust	38.16	kJ/mol	348.50	NIST Webbook
sfust	109.50	J/mol×K	348.50	NIST Webbook
sfust	40.54	J/mol×K	170.20	NIST Webbook

Sources

Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons:	https://www.doi.org/10.1021/je300504f
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=C307595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume