Methane, fluorotrinitro-

Other names: Fluorotrinitromethane
Inchi: InChI=1S/CFN3O6/c2-1(3(6)7,4(8)9)5(10)11
InchiKey: IHOVZLJULZIGOW-UHFFFAOYSA-N
Formula: CFN3O6
SMILES: O=[N+]([O-])C(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 169.03
CAS: 1840-42-2

Physical Properties

Property code	Value	Unit	Source
chl	-3336.60 ± 2.00	kJ/mol	NIST Webbook
gf	-127.78	kJ/mol	Joback Method
hf	-301.11	kJ/mol	Joback Method
hfl	-220.20 ± 2.00	kJ/mol	NIST Webbook
hfus	28.09	kJ/mol	Joback Method
hvap	34.70 ± 0.42	kJ/mol	NIST Webbook
log10ws	-1.94		Crippen Method
logp	-0.603		Crippen Method
mcvol	78.980	ml/mol	McGowan Method
pc	5880.91	kPa	Joback Method
tb	673.84	K	Joback Method
tc	955.10	K	Joback Method
tf	244.15 ± 0.10	K	NIST Webbook
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.18	J/mol×K	673.84	Joback Method
cpg	200.97	J/mol×K	720.72	Joback Method
cpg	205.07	J/mol×K	767.59	Joback Method
cpg	208.57	J/mol×K	814.47	Joback Method
cpg	211.54	J/mol×K	861.35	Joback Method
cpg	214.09	J/mol×K	908.22	Joback Method

cpg	216.29	J/mol×K	955.10	Joback Method
hvapt	34.20	kJ/mol	316.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63754e+01
Coeff. B	-4.19317e+03
Temperature range (K), min.	260.64
Temperature range (K), max.	378.99

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1840422&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
vc:	Critical Volume