Fluorodinitrophenylmethane

Other names: Fluorodinitrophenylethane
Inchi: InChI=1S/C7H5FN2O4/c8-7(9(11)12,10(13)14)6-4-2-1-3-5-6/h1-5H
InchiKey: NPRRCIKUIFRPTB-UHFFFAOYSA-N
Formula: C7H5FN2O4
SMILES: O=[N+]([O-])C(F)(c1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]: 200.12
CAS: 17003-70-2

Physical Properties

Property code	Value	Unit	Source
chl	-3410.80 ± 1.70	kJ/mol	NIST Webbook
gf	-0.40	kJ/mol	Joback Method
hf	-185.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-238.00 ± 2.00	kJ/mol	NIST Webbook
hfus	26.32	kJ/mol	Joback Method
hvap	52.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.04		Crippen Method
logp	1.320		Crippen Method
mcvol	122.340	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	685.96	K	Joback Method
tc	961.91	K	Joback Method
tf	485.30	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.44	J/mol×K	915.92	Joback Method
cpg	314.87	J/mol×K	685.96	Joback Method
cpg	324.55	J/mol×K	731.95	Joback Method
cpg	333.12	J/mol×K	777.94	Joback Method
cpg	340.71	J/mol×K	823.94	Joback Method
cpg	347.44	J/mol×K	869.93	Joback Method

cpg	358.84	J/mol×K	961.91	Joback Method
hvapt	52.80	kJ/mol	345.50	NIST Webbook

Sources

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=C17003702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume