Benzene, 1-fluoro-2,4-dinitro-

Other names:	Dinitrofluorobenzene
	DFB
	DNFB
	Fluoro-2,4-dinitrobenzene
	Fluorodinitrobenzene
	FDNB
	1-Fluoro-2,4-dinitrobenzene
	2,4-Dinitro-1-fluorobenzene
	2,4-Dinitrobenzenefluoride
	2,4-Dinitrofluorobenzene
	2,4-Dinitrophenyl fluoride
	Benzene, 2,4-dinitro-1-fluoro-
	1,2,4-Fluorodinitrobenzene
	2,4-DNFB
	NSC 33519
Inchi:	InChI=1S/C6H3FN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H
InchiKey:	LOTKRQAVGJMPNV-UHFFFAOYSA-N
Formula:	C6H3FN2O4
SMILES:	O=[N+]([O-])c1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	186.10
CAS:	70-34-8

Physical Properties

Property code	Value	Unit	Source
chs	-2800.10	kJ/mol	NIST Webbook
gf	-30.92	kJ/mol	Joback Method
hf	-171.21	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	64.91	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.642		Crippen Method
mcvol	108.250	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	676.27	K	Joback Method
tc	943.68	K	Joback Method
tf	496.65	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.31	J/mol×K	676.27	Joback Method
cpg	268.52	J/mol×K	720.84	Joback Method
cpg	275.94	J/mol×K	765.41	Joback Method
cpg	282.62	J/mol×K	809.97	Joback Method
cpg	288.61	J/mol×K	854.54	Joback Method
cpg	293.93	J/mol×K	899.11	Joback Method
cpg	298.65	J/mol×K	943.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	3.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70348&Units=SI
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

Legend

chs: Standard solid enthalpy of combustion
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume