Phenol, 2,6-dinitro-4-fluoro-

Inchi: InChI=1S/C6H3FN2O5/c7-3-1-4(8(11)12)6(10)5(2-3)9(13)14/h1-2,10H
InchiKey: MDOWEUXXLVBZIU-UHFFFAOYSA-N
Formula: C6H3FN2O5
SMILES: O=[N+]([O-])c1cc(F)cc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 202.10
CAS: 364-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-185.54	kJ/mol	Joback Method
hf	-348.52	kJ/mol	Joback Method
hfus	36.14	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.348		Crippen Method
mcvol	114.120	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
tb	756.89	K	Joback Method
tc	1030.09	K	Joback Method
tf	608.37	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.53	J/mol×K	756.89	Joback Method
cpg	300.38	J/mol×K	802.42	Joback Method
cpg	306.76	J/mol×K	847.96	Joback Method
cpg	312.79	J/mol×K	893.49	Joback Method
cpg	318.60	J/mol×K	939.02	Joback Method
cpg	324.29	J/mol×K	984.56	Joback Method
cpg	330.00	J/mol×K	1030.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C364329&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

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
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