Benzene, 1,5-difluoro-2,4-dinitro-

Other names:	1,3-Difluoro-4,6-dinitrobenzene
	1,5-Difluoro-2,4-dinitrobenzene
	4,6-Difluoro-1,3-dinitrobenzene
	2,4-Dinitro-1,5-difluorobenzene
	Benzene, 1,3-difluoro-4,6-dinitro-
Inchi:	InChI=1S/C6H2F2N2O4/c7-3-1-4(8)6(10(13)14)2-5(3)9(11)12/h1-2H
InchiKey:	VILFTWLXLYIEMV-UHFFFAOYSA-N
Formula:	C6H2F2N2O4
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(F)cc1F
Mol. weight [g/mol]:	204.09
CAS:	327-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-235.36	kJ/mol	Joback Method
hf	-378.79	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	64.76	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	1.781		Crippen Method
mcvol	110.020	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	680.52	K	Joback Method
tc	935.78	K	Joback Method
tf	509.76	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.43	J/mol×K	680.52	Joback Method
cpg	273.99	J/mol×K	723.06	Joback Method
cpg	280.87	J/mol×K	765.61	Joback Method
cpg	287.09	J/mol×K	808.15	Joback Method

cpg	292.69	J/mol×K	850.69	Joback Method
cpg	297.70	J/mol×K	893.23	Joback Method
cpg	302.14	J/mol×K	935.78	Joback Method

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=C327924&Units=SI

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