3,4-Difluoronitrobenzene

Other names:	Benzene, 1,2-difluoro-4-nitro-
	1,2-Difluoro-4-nitrobenzene
Inchi:	InChI=1S/C6H3F2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H
InchiKey:	RUBQQRMAWLSCCJ-UHFFFAOYSA-N
Formula:	C6H3F2NO2
SMILES:	O=[N+]([O-])c1ccc(F)c(F)c1
Mol. weight [g/mol]:	159.09
CAS:	369-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-261.28	kJ/mol	Joback Method
hf	-356.56	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	47.51	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.873		Crippen Method
mcvol	92.600	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	523.70	K	Joback Method
tc	753.60	K	Joback Method
tf	353.63	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.39	J/mol×K	523.70	Joback Method
cpg	203.84	J/mol×K	562.02	Joback Method
cpg	211.70	J/mol×K	600.33	Joback Method
cpg	219.01	J/mol×K	638.65	Joback Method
cpg	225.78	J/mol×K	676.96	Joback Method
cpg	232.03	J/mol×K	715.28	Joback Method
cpg	237.80	J/mol×K	753.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.00	K	2.70	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=C369346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume