

2,5-Difluoronitrobenzene

Other names:	Benzene, 1,4-difluoro-2-nitro- 1,4-Difluoro-2-nitrobenzene
Inchi:	InChI=1S/C6H3F2NO2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H
InchiKey:	XNJAYQHWXYJBBD-UHFFFAOYSA-N
Formula:	C6H3F2NO2
SMILES:	O=[N+](O-)c1cc(F)ccc1F
Mol. weight [g/mol]:	159.09
CAS:	364-74-9

Physical Properties

Property code	Value	Unit	Source
chs	-2816.00	kJ/mol	NIST Webbook
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	479.60	K	NIST Webbook
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/molxK	523.70	Joback Method
cpg	203.84	J/molxK	562.02	Joback Method
cpg	211.70	J/molxK	600.33	Joback Method
cpg	219.01	J/molxK	638.65	Joback Method
cpg	225.78	J/molxK	676.96	Joback Method
cpg	232.03	J/molxK	715.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C364749&Units=SI

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

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