

Benzenamine, 4-fluoro-3-nitro-

Other names:	Aniline, 4-fluoro-3-nitro- 3-Nitro-4-fluoroaniline 4-Fluoro-3-nitroaniline 4-Fluoro-3-nitrobenzenamine 4-F-3NA
Inchi:	InChI=1S/C6H5FN2O2/c7-5-2-1-4(8)3-6(5)9(10)11/h1-3H,8H2
InchiKey:	LLIOADBCFIXIEU-UHFFFAOYSA-N
Formula:	C6H5FN2O2
SMILES:	<chem>Nc1ccc(F)c([N+](=O)[O-])c1</chem>
Mol. weight [g/mol]:	156.11
CAS:	364-76-1

Physical Properties

Property code	Value	Unit	Source
chs	-3083.00	kJ/mol	NIST Webbook
gf	-0.02	kJ/mol	Joback Method
hf	-126.66	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.316		Crippen Method
mcvol	100.810	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	596.96	K	Joback Method
tc	847.98	K	Joback Method
tf	436.30	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.87	J/molxK	596.96	Joback Method
cpg	241.83	J/molxK	638.80	Joback Method
cpg	250.09	J/molxK	680.63	Joback Method

cpg	257.69	J/mol×K	722.47	Joback Method
cpg	264.65	J/mol×K	764.31	Joback Method
cpg	271.01	J/mol×K	806.14	Joback Method
cpg	276.80	J/mol×K	847.98	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=C364761&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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