2-Fluoro-5-nitroaniline

Other names: Benzenamine, 2-fluoro-5-nitro-
Aniline, 2-fluoro-5-nitro-
1-Amino-2-fluoro-5-nitrobenzene
Inchi: InChI=1S/C6H5FN2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2
InchiKey: KJVBJICWGQIMOZ-UHFFFAOYSA-N
Formula: C6H5FN2O2
SMILES: Nc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]: 156.11
CAS: 369-36-8

Physical Properties

Property code	Value	Unit	Source
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/mol×K	596.96	Joback Method
cpg	241.83	J/mol×K	638.80	Joback Method
cpg	250.09	J/mol×K	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C369368&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