3-Chloro-4-fluoronitrobenzene

Other names: Benzene, 2-chloro-1-fluoro-4-nitro-
2-Chloro-1-fluoro-4-nitrobenzene
Inchi: InChI=1S/C6H3ClFNO2/c7-5-3-4(9(10)11)1-2-6(5)8/h1-3H
InchiKey: DPHCXXYPSYMICK-UHFFFAOYSA-N
Formula: C6H3ClFNO2
SMILES: O=[N+]([O-])c1ccc(F)c(Cl)c1
Mol. weight [g/mol]: 175.54
CAS: 350-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-78.40	kJ/mol	Joback Method
hf	-176.19	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.387		Crippen Method
mcvol	103.070	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	561.86	K	Joback Method
tc	808.99	K	Joback Method
tf	382.96	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.13	J/mol×K	561.86	Joback Method
cpg	215.31	J/mol×K	603.05	Joback Method
cpg	222.86	J/mol×K	644.24	Joback Method
cpg	229.79	J/mol×K	685.43	Joback Method
cpg	236.15	J/mol×K	726.62	Joback Method
cpg	241.96	J/mol×K	767.81	Joback Method
cpg	247.25	J/mol×K	808.99	Joback Method

Sources

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=C350301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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