

3-FLUORO-4-NITROPHENOL

Other names:	3-Fluoro-4-nitrophenol
Inchi:	InChI=1S/C6H4FNO3/c7-5-3-4(9)1-2-6(5)8(10)11/h1-3,9H
InchiKey:	CSSGKHVRDGATJL-UHFFFAOYSA-N
Formula:	C6H4FNO3
SMILES:	O=[N+]([O-])c1ccc(O)cc1F
Mol. weight [g/mol]:	157.10

Physical Properties

Property code	Value	Unit	Source
hf	-289.37	kJ/mol	Cheméo Relay (1.0)
hfus	25.17	kJ/mol	Joback Method
hvap	79.12	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-1.90		Cheméo Relay (1.0)
logp	1.440		Crippen Method
mcvol	96.700	ml/mol	McGowan Method
tb	518.67	K	Cheméo Relay (1.0)
tf	357.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.12	J/mol×K	600.07	Joback Method
cpg	234.01	J/mol×K	642.17	Joback Method
cpg	241.21	J/mol×K	684.26	Joback Method
cpg	247.81	J/mol×K	726.36	Joback Method
cpg	253.92	J/mol×K	768.45	Joback Method
cpg	259.63	J/mol×K	810.55	Joback Method
cpg	265.04	J/mol×K	852.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394412&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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