

Benzene, 4-fluoro-2-methyl-1-nitro-

Other names:	Toluene, 5-fluoro-2-nitro- 2-Methyl-4-fluoronitrobenzene 3-Fluoro-6-nitrotoluene 3-Methyl-4-nitrofluorobenzene 5-Fluoro-2-nitrotoluene
Inchi:	InChI=1S/C7H6FNO2/c1-5-4-6(8)2-3-7(5)9(10)11/h2-4H,1H3
InchiKey:	JHFOWEGCZWLHNW-UHFFFAOYSA-N
Formula:	C7H6FNO2
SMILES:	Cc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	155.13
CAS:	446-33-3

Physical Properties

Property code	Value	Unit	Source
ea	1.01 ± 0.05	eV	NIST Webbook
gf	-58.05	kJ/mol	Joback Method
hf	-181.09	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	50.55	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.042		Crippen Method
mcvol	104.920	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	547.31	K	Joback Method
tc	785.21	K	Joback Method
tf	364.31	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.86	J/mol×K	547.31	Joback Method
cpg	239.05	J/mol×K	586.96	Joback Method
cpg	248.55	J/mol×K	626.61	Joback Method

cpg	257.38	J/mol×K	666.26	Joback Method
cpg	265.58	J/mol×K	705.91	Joback Method
cpg	273.16	J/mol×K	745.56	Joback Method
cpg	280.17	J/mol×K	785.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	1.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C446333&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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