3-Fluoro-4-nitrotoluene

Other names: Benzene, 2-fluoro-4-methyl-1-nitro-
Inchi: InChI=1S/C7H6FNO2/c1-5-2-3-7(9(10)11)6(8)4-5/h2-4H,1H3
InchiKey: WZMOWQCNPFDWPA-UHFFFAOYSA-N
Formula: C7H6FNO2
SMILES: Cc1ccc([N+](=O)[O-])c(F)c1
Mol. weight [g/mol]: 155.13
CAS: 446-34-4

Physical Properties

Property code	Value	Unit	Source
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	0.40	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C446344&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume