4-Fluoro-3-nitrobenzoic acid

Other names:	Benzoic acid, 4-fluoro-3-nitro-
	p-Fluoro-3-nitrobenzoic acid
Inchi:	InChI=1S/C7H4FNO4/c8-5-2-1-4(7(10)11)3-6(5)9(12)13/h1-3H,(H,10,11)
InchiKey:	BOJWTAQWPVBIPG-UHFFFAOYSA-N
Formula:	C7H4FNO4
SMILES:	O=C(O)c1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	185.11
CAS:	453-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-323.79	kJ/mol	Joback Method
hf	-445.90	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Joback Method
log10ws	-1.58		Aqueous Solubility Prediction Method
logp	1.432		Crippen Method
mcvol	112.360	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	693.36	K	Joback Method
tc	918.05	K	Joback Method
tf	475.06	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.47	J/mol×K	693.36	Joback Method
cpg	281.48	J/mol×K	730.81	Joback Method
cpg	287.92	J/mol×K	768.26	Joback Method
cpg	293.84	J/mol×K	805.71	Joback Method
cpg	299.24	J/mol×K	843.15	Joback Method
cpg	304.16	J/mol×K	880.60	Joback Method

cpg	308.61	J/mol×K	918.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C453714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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