Benzoic acid, 4-nitro-, methyl ester

Other names:	4-Nitrobenzoic acid methyl ester
	Benzoic acid, p-nitro-, methyl ester
	Methyl 4-nitrobenzoate
	Methyl ester of 4-Nitrobenzoic acid
	Methyl p-nitrobenzoate
	Methyl para-nitrobenzoate
	p-Nitrobenzoic acid methyl ester
Inchi:	InChI=1S/C8H7NO4/c1-13-8(10)6-2-4-7(5-3-6)9(11)12/h2-5H,1H3
InchiKey:	YOJAHJGBFDPSDI-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	COC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	181.15
CAS:	619-50-1

Physical Properties

Property code	Value	Unit	Source
affp	813.20	kJ/mol	NIST Webbook
basg	782.30	kJ/mol	NIST Webbook
ea	1.47 ± 0.09	eV	NIST Webbook
ea	1.46 ± 0.09	eV	NIST Webbook
gf	-79.11	kJ/mol	Joback Method
hf	-287.00 ± 11.00	kJ/mol	NIST Webbook
hfl	-387.20 ± 1.30	kJ/mol	NIST Webbook
hfus	24.28	kJ/mol	Joback Method
hvap	100.00 ± 10.00	kJ/mol	NIST Webbook
ie	9.70	eV	NIST Webbook
log10ws	-3.04		Aqueous Solubility Prediction Method
logp	1.381		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1427.00		NIST Webbook

rinpol	1449.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2314.00		NIST Webbook
tb	642.23	K	Joback Method
tc	889.97	K	Joback Method
tf	368.82	K	Aqueous Solubility Prediction Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.26	J/mol×K	642.23	Joback Method
cpg	308.88	J/mol×K	683.52	Joback Method
cpg	318.68	J/mol×K	724.81	Joback Method
cpg	327.67	J/mol×K	766.10	Joback Method
cpg	335.88	J/mol×K	807.39	Joback Method
cpg	343.31	J/mol×K	848.68	Joback Method
cpg	349.99	J/mol×K	889.97	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619501&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity

ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume