3-Hydroxy-4-methoxynitrobenzene

Other names:	5-Nitroguaiacol
	Phenol, 2-methoxy-5-nitro-
	2-Methoxy-5-nitrophenol
Inchi:	InChI=1S/C7H7NO4/c1-12-7-3-2-5(8(10)11)4-6(7)9/h2-4,9H,1H3
InchiKey:	KXKCTSZYNCDFFG-UHFFFAOYSA-N
Formula:	C7H7NO4
SMILES:	COc1ccc([N+](=O)[O-])cc1O
Mol. weight [g/mol]:	169.13
CAS:	636-93-1

Physical Properties

Property code	Value	Unit	Source
gf	-113.23	kJ/mol	Joback Method
hf	-283.04	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.309		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	646.10	K	Joback Method
tc	901.50	K	Joback Method
tf	485.15	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.54	J/mol×K	646.10	Joback Method
cpg	292.99	J/mol×K	688.67	Joback Method
cpg	301.75	J/mol×K	731.23	Joback Method
cpg	309.89	J/mol×K	773.80	Joback Method
cpg	317.50	J/mol×K	816.36	Joback Method
cpg	324.65	J/mol×K	858.93	Joback Method

cpg	331.41	J/mol×K	901.50	Joback Method

Sources

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=C636931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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