Ethanone, 1-(4-hydroxy-3-nitrophenyl)-

Other names:	4'-Hydroxy-3'-Nitro acetophenone
	4-Hydroxy-3-nitroacetophenone
Inchi:	InChI=1S/C8H7NO4/c1-5(10)6-2-3-8(11)7(4-6)9(12)13/h2-4,11H,1H3
InchiKey:	MMNKVWGVSHRIJL-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	CC(=O)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	181.15
CAS:	6322-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-128.73	kJ/mol	Joback Method
hf	-284.04	kJ/mol	Joback Method
hfus	28.87	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.503		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	700.43	K	Joback Method
tc	959.94	K	Joback Method
tf	524.12	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.47	J/mol×K	700.43	Joback Method
cpg	324.55	J/mol×K	743.68	Joback Method
cpg	332.96	J/mol×K	786.93	Joback Method
cpg	340.79	J/mol×K	830.18	Joback Method
cpg	348.17	J/mol×K	873.43	Joback Method
cpg	355.19	J/mol×K	916.69	Joback Method
cpg	361.98	J/mol×K	959.94	Joback Method

Sources

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=C6322561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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