Benzophenone, 2-hydroxy-5-nitro-

Inchi: InChI=1S/C13H9NO4/c15-12-7-6-10(14(17)18)8-11(12)13(16)9-4-2-1-3-5-9/h1-8,15H
InchiKey: YHRILHYQNVLOEQ-UHFFFAOYSA-N
Formula: C13H9NO4
SMILES: O=C(c1ccccc1)c1cc([N+](=O)[O-])ccc1O
Mol. weight [g/mol]: 243.21
CAS: 18803-19-5

Physical Properties

Property code	Value	Unit	Source
gf	25.78	kJ/mol	Joback Method
hf	-150.71	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	86.10	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.531		Crippen Method
mcvol	171.370	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	841.51	K	Joback Method
tc	1118.60	K	Joback Method
tf	606.89	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.56	J/mol×K	841.51	Joback Method
cpg	484.20	J/mol×K	887.69	Joback Method
cpg	494.15	J/mol×K	933.87	Joback Method
cpg	503.61	J/mol×K	980.05	Joback Method
cpg	512.76	J/mol×K	1026.24	Joback Method
cpg	521.78	J/mol×K	1072.42	Joback Method
cpg	530.85	J/mol×K	1118.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18803195&Units=SI
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

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