Benzophenone, 2,4-dihydroxy-4'-nitro-

Inchi: InChI=1S/C13H9NO5/c15-10-5-6-11(12(16)7-10)13(17)8-1-3-9(4-2-8)14(18)19/h1-7,15-1
InchiKey: SGDKXQGGKPQZGD-UHFFFAOYSA-N
Formula: C13H9NO5
SMILES: O=C(c1ccc([N+](=O)[O-])cc1)c1ccc(O)cc1O
Mol. weight [g/mol]: 259.21
CAS: 6994-40-7

Physical Properties

Property code	Value	Unit	Source
gf	-128.84	kJ/mol	Joback Method
hf	-328.02	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	99.11	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.237		Crippen Method
mcvol	177.240	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	922.13	K	Joback Method
tc	1202.77	K	Joback Method
tf	718.61	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.70	J/mol×K	922.13	Joback Method
cpg	522.64	J/mol×K	968.90	Joback Method
cpg	533.79	J/mol×K	1015.68	Joback Method
cpg	545.41	J/mol×K	1062.45	Joback Method
cpg	557.79	J/mol×K	1109.22	Joback Method
cpg	571.20	J/mol×K	1155.99	Joback Method
cpg	585.91	J/mol×K	1202.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6994407&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