

Methanone, (2,4-dihydroxyphenyl)(4-hydroxyphenyl)-

Other names:	Benzophenone, 2,4,4'-trihydroxy- 2,4-Dihydroxyphenyl p-hydroxybenzyl ketone 2,4,4'-Trihydroxybenzophenone
Inchi:	InChI=1S/C13H10O4/c14-9-3-1-8(2-4-9)13(17)11-6-5-10(15)7-12(11)16/h1-7,14-16H
InchiKey:	OKJFKPFBSPZTAH-UHFFFAOYSA-N
Formula:	C13H10O4
SMILES:	O=C(c1ccc(O)cc1)c1ccc(O)cc1O
Mol. weight [g/mol]:	230.22
CAS:	1470-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-309.38	kJ/mol	Joback Method
hf	-483.10	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	94.87	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.034		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
tb	845.93	K	Joback Method
tc	1116.79	K	Joback Method
tf	674.20	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.29	J/molxK	845.93	Joback Method
cpg	481.19	J/molxK	891.07	Joback Method
cpg	492.36	J/molxK	936.22	Joback Method
cpg	504.13	J/molxK	981.36	Joback Method
cpg	516.82	J/molxK	1026.50	Joback Method
cpg	530.75	J/molxK	1071.65	Joback Method

cpg	546.24	J/molxK	1116.79	Joback Method
dvisc	0.0000005	Paxs	674.20	Joback Method
dvisc	0.0000003	Paxs	702.82	Joback Method
dvisc	0.0000002	Paxs	731.44	Joback Method
dvisc	0.0000001	Paxs	760.07	Joback Method
dvisc	6.7691086e-08	Paxs	788.69	Joback Method
dvisc	4.4620809e-08	Paxs	817.31	Joback Method
dvisc	3.0254579e-08	Paxs	845.93	Joback Method
hfust	31.30	kJ/mol	482.60	NIST Webbook

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=C1470797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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