

METHANONE, (2-HYDROXY-5-METHOXYPHENYL)PHENYL-

Other names:2'-Hydroxy-5'-methoxybenzophenone

Methanone, (2-hydroxy-5-methoxyphenyl)phenyl-

Inchi:InChI=1S/C14H12O3/c1-17-11-7-8-13(15)12(9-11)14(16)10-5-3-2-4-6-10/h2-9,15H,1H3

InchiKey:RIFCEURUCJPMOQ-UHFFFAOYSA-N

Formula:C14H12O3

SMILES:COc1ccc(O)c(C(=O)c2ccccc2)c1

Mol. weight [g/mol]:228.25

Physical Properties

Property code	Value	Unit	Source
af	0.7121		Cheméo Relay (1.0)
hf	-284.02	kJ/mol	Cheméo Relay (1.0)
hfus	28.28	kJ/mol	Joback Method
hvap	96.01	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-3.50		Cheméo Relay (1.0)
logp	2.632		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	619.53	K	Cheméo Relay (1.0)
tc	899.20	K	Cheméo Relay (1.0)
tf	361.51	K	Cheméo Relay (1.0)
vc	0.621	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.89	J/mol×K	734.97	Joback Method
cpg	475.85	J/mol×K	776.76	Joback Method
cpg	487.84	J/mol×K	818.55	Joback Method
cpg	498.98	J/mol×K	860.34	Joback Method
cpg	509.38	J/mol×K	902.13	Joback Method
cpg	519.15	J/mol×K	943.92	Joback Method
cpg	528.39	J/mol×K	985.71	Joback Method

dvisc	0.0002250	Pa×s	496.78	Joback Method
dvisc	0.0001147	Pa×s	536.48	Joback Method
dvisc	0.0000641	Pa×s	576.18	Joback Method
dvisc	0.0000387	Pa×s	615.88	Joback Method
dvisc	0.0000248	Pa×s	655.57	Joback Method
dvisc	0.0000167	Pa×s	695.27	Joback Method
dvisc	0.0000118	Pa×s	734.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14770968&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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