

2-hydroxyl-3,4,6-trimethoxy-acetophenone

Inchi:	InChI=1S/C11H14O5/c1-6(12)9-7(14-2)5-8(15-3)11(16-4)10(9)13/h5,13H,1-4H3
InchiKey:	WLTFZNFPHXCIAO-UHFFFAOYSA-N
Formula:	C11H14O5
SMILES:	COc1cc(OC)c(C(C)=O)c(O)c1OC
Mol. weight [g/mol]:	226.23

Physical Properties

Property code	Value	Unit	Source
gf	-473.28	kJ/mol	Joback Method
hf	-754.80	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.621		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	694.45	K	Joback Method
tc	911.29	K	Joback Method
tf	506.05	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.63	J/molxK	694.45	Joback Method
cpg	497.65	J/molxK	875.15	Joback Method
cpg	488.08	J/molxK	839.01	Joback Method
cpg	477.90	J/molxK	802.87	Joback Method
cpg	467.11	J/molxK	766.73	Joback Method
cpg	455.69	J/molxK	730.59	Joback Method
cpg	506.61	J/molxK	911.29	Joback Method
dvisc	0.0000117	Paxs	694.45	Joback Method

dvisc	0.0000158	Paxs	663.05	Joback Method
dvisc	0.0000218	Paxs	631.65	Joback Method
dvisc	0.0000313	Paxs	600.25	Joback Method
dvisc	0.0000467	Paxs	568.85	Joback Method
dvisc	0.0000730	Paxs	537.45	Joback Method
dvisc	0.0001207	Paxs	506.05	Joback Method

Sources

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=R301527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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