Propiosyringone

Other names:	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)
	1-(4-Hydroxy-3,5-dimethoxyphenyl)-1-propanone (propiosyringone)
	1-(4-hydroxy-3,5-dimethoxyphenyl)propanone (propiosyringone)
	1-(4-hydroxy-3,5-dimethoxyphenyl)propanone
Inchi:	InChI=1S/C11H14O4/c1-4-8(12)7-5-9(14-2)11(13)10(6-7)15-3/h5-6,13H,4H2,1-3H3
InchiKey:	CXCPJZXJNRBTGF-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	CCC(=O)c1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]:	210.23
CAS:	5650-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-358.65	kJ/mol	Joback Method
hf	-611.11	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.002		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	667.05	K	Joback Method
tc	885.56	K	Joback Method
tf	471.30	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.53	J/mol×K	667.05	Joback Method
cpg	432.84	J/mol×K	703.47	Joback Method
cpg	444.47	J/mol×K	739.89	Joback Method

cpg	455.46	J/mol×K	776.31	Joback Method
cpg	465.83	J/mol×K	812.72	Joback Method
cpg	475.62	J/mol×K	849.14	Joback Method
cpg	484.86	J/mol×K	885.56	Joback Method
dvisc	0.0002436	Pa×s	471.30	Joback Method
dvisc	0.0001353	Pa×s	503.93	Joback Method
dvisc	0.0000807	Pa×s	536.55	Joback Method
dvisc	0.0000511	Pa×s	569.17	Joback Method
dvisc	0.0000340	Pa×s	601.80	Joback Method
dvisc	0.0000236	Pa×s	634.42	Joback Method
dvisc	0.0000170	Pa×s	667.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5650431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
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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