2-Butanone, 4-(4-hydroxy-3-methoxyphenyl)-

Other names:	(4-Hydroxy-3-methoxyphenyl)ethyl methyl ketone
	[0]-Paradol
	Vanillylacetone
	Zingerone
	Zingiberone
	3-Methoxy-4-hydroxybenzylacetone
	4-(4-Hydroxy-3-methoxyphenyl)-2-butanone
	4-Hydroxy-3-methoxybenzylacetone
	Gingerone
	NSC 15335
	zingerone [3-(4-hydroxy-3-methoxyphenyl)butan-2-one]
	Zingerone (vanillyl acetone)
	4-(4-hydroxy-3-methoxyphenyl)butan-2-one
Inchi:	InChI=1S/C11H14O3/c1-8(12)3-4-9-5-6-10(13)11(7-9)14-2/h5-7,13H,3-4H2,1-2H3
InchiKey:	OJYLAHXKWMRDGS-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	COc1cc(CCC(C)=O)ccc1O
Mol. weight [g/mol]:	194.23
CAS:	122-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-244.02	kJ/mol	Joback Method
hf	-467.42	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.922		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1656.00		NIST Webbook

rinpol	1653.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1635.00		NIST Webbook
ripol	2826.00		NIST Webbook
ripol	2790.00		NIST Webbook
ripol	2790.00		NIST Webbook
ripol	2779.00		NIST Webbook
ripol	2751.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2779.00		NIST Webbook
ripol	2829.00		NIST Webbook
ripol	2829.00		NIST Webbook
ripol	2829.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2786.00		NIST Webbook
tb	639.65	K	Joback Method
tc	859.98	K	Joback Method
tf	436.55	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.49	J/mol×K	639.65	Joback Method
cpg	453.72	J/mol×K	823.26	Joback Method
cpg	443.76	J/mol×K	786.54	Joback Method
cpg	433.22	J/mol×K	749.81	Joback Method
cpg	422.03	J/mol×K	713.09	Joback Method
cpg	410.14	J/mol×K	676.37	Joback Method
cpg	463.15	J/mol×K	859.98	Joback Method
dvisc	0.0000247	Pa×s	639.65	Joback Method
dvisc	0.0000357	Pa×s	605.80	Joback Method
dvisc	0.0000539	Pa×s	571.95	Joback Method
dvisc	0.0000856	Pa×s	538.10	Joback Method
dvisc	0.0001447	Pa×s	504.25	Joback Method
dvisc	0.0002638	Pa×s	470.40	Joback Method
dvisc	0.0005280	Pa×s	436.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122485&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume