3-Buten-2-one, 4-(4-hydroxy-3-methoxyphenyl)-

Other names: (O)-Dehydroparadol
(O)-Paradol, dehydro-
Dehydrozingerone
Feruloylmethane
3-Methoxy-4-hydroxybenzalacetone
4-Hydroxy-3-methoxystyryl methyl ketone
4-(4-Hydroxy-3-methoxyphenyl)-3-buten-2-one
Methyl-3-methoxy-4-hydroxy styryl ketone
MHSK
4-Hydroxy-3-methoxybenzylideneacetone
Dehydro(O)-paradol
NSC 26613
NSC 4019
NSC 44708
NSC 5316
Vanillalacetone
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one

Inchi: InChI=1S/C11H12O3/c1-8(12)3-4-9-5-6-10(13)11(7-9)14-2/h3-7,13H,1-2H3/b4-3+

InchiKey: AFWKBSMFXWNGRE-ONEGZZNKSA-N

Formula: C11H12O3

SMILES: COc1cc(C=CC(C)=O)ccc1O

Mol. weight [g/mol]: 192.21

CAS: 1080-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-163.80	kJ/mol	Joback Method
hf	-350.20	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.003		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	643.81	K	Joback Method

tc	873.35	K	Joback Method
tf	431.47	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.57	J/mol×K	643.81	Joback Method
cpg	428.50	J/mol×K	835.10	Joback Method
cpg	419.14	J/mol×K	796.84	Joback Method
cpg	409.25	J/mol×K	758.58	Joback Method
cpg	398.75	J/mol×K	720.32	Joback Method
cpg	387.55	J/mol×K	682.07	Joback Method
cpg	437.40	J/mol×K	873.35	Joback Method
dvisc	0.0000207	Pa×s	643.81	Joback Method
dvisc	0.0000303	Pa×s	608.42	Joback Method
dvisc	0.0000463	Pa×s	573.03	Joback Method
dvisc	0.0000748	Pa×s	537.64	Joback Method
dvisc	0.0001295	Pa×s	502.25	Joback Method
dvisc	0.0002436	Pa×s	466.86	Joback Method
dvisc	0.0005083	Pa×s	431.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1080122&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

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