4-Hexen-3-one, 5-methyl-2-(3-hydroxy-4-methylphenyl)

Inchi: InChI=1S/C14H18O2/c1-9(2)7-14(16)11(4)12-6-5-10(3)13(15)8-12/h5-8,11,15H,1-4H3
InchiKey: WZHLEYQOLDOTEY-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: CC(C)=CC(=O)C(C)c1ccc(C)c(O)c1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	-44.53	kJ/mol	Joback Method
hf	-294.97	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.339		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	689.47	K	Joback Method
tc	917.49	K	Joback Method
tf	414.09	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.40	J/mol×K	689.47	Joback Method
cpg	516.03	J/mol×K	727.47	Joback Method
cpg	529.77	J/mol×K	765.48	Joback Method
cpg	542.72	J/mol×K	803.48	Joback Method
cpg	554.98	J/mol×K	841.48	Joback Method
cpg	566.66	J/mol×K	879.49	Joback Method
cpg	577.89	J/mol×K	917.49	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=R400129&Units=SI

Legend

cpg:	Ideal gas heat capacity
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