2-(2-Hydroxy-4-methyl-phenyl)-pentan-3-one

Inchi: InChI=1S/C12H16O2/c1-4-11(13)9(3)10-6-5-8(2)7-12(10)14/h5-7,9,14H,4H2,1-3H3
InchiKey: XKKGHYTULRMGQQ-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CCC(=O)C(C)c1ccc(C)cc1O
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-133.04	kJ/mol	Joback Method
hf	-361.12	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.783		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
ripol	2620.00		NIST Webbook
ripol	2620.00		NIST Webbook
tb	639.67	K	Joback Method
tc	863.30	K	Joback Method
tf	410.59	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.73	J/mol×K	639.67	Joback Method
cpg	436.61	J/mol×K	676.94	Joback Method
cpg	449.62	J/mol×K	714.21	Joback Method
cpg	461.84	J/mol×K	751.48	Joback Method
cpg	473.33	J/mol×K	788.76	Joback Method
cpg	484.20	J/mol×K	826.03	Joback Method
cpg	494.50	J/mol×K	863.30	Joback Method
dvisc	0.0010385	Pa×s	410.59	Joback Method

dvisc	0.0004332	Pa×s	448.77	Joback Method
dvisc	0.0002073	Pa×s	486.95	Joback Method
dvisc	0.0001104	Pa×s	525.13	Joback Method
dvisc	0.0000640	Pa×s	563.31	Joback Method
dvisc	0.0000398	Pa×s	601.49	Joback Method
dvisc	0.0000262	Pa×s	639.67	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=R326071&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume