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

Inchi: InChI=1S/C11H14O2/c1-7-4-5-10(11(13)6-7)8(2)9(3)12/h4-6,8,13H,1-3H3
InchiKey: YWKYLGVKGIAHDU-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC(=O)C(C)c1ccc(C)cc1O
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-141.46	kJ/mol	Joback Method
hf	-340.48	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.393		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
ripol	2605.00		NIST Webbook
ripol	2605.00		NIST Webbook
tb	616.79	K	Joback Method
tc	844.69	K	Joback Method
tf	399.32	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.96	J/mol×K	616.79	Joback Method
cpg	387.15	J/mol×K	654.77	Joback Method
cpg	399.48	J/mol×K	692.76	Joback Method
cpg	411.03	J/mol×K	730.74	Joback Method
cpg	421.86	J/mol×K	768.73	Joback Method
cpg	432.07	J/mol×K	806.71	Joback Method
cpg	441.73	J/mol×K	844.69	Joback Method
dvisc	0.0012402	Pa×s	399.32	Joback Method

dvisc	0.0005250	Pa×s	435.56	Joback Method
dvisc	0.0002536	Pa×s	471.81	Joback Method
dvisc	0.0001359	Pa×s	508.05	Joback Method
dvisc	0.0000792	Pa×s	544.30	Joback Method
dvisc	0.0000493	Pa×s	580.54	Joback Method
dvisc	0.0000325	Pa×s	616.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326140&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume