5-phenyl-2-hydroxy-3-pentanone

Inchi: InChI=1S/C11H14O2/c1-9(12)11(13)8-7-10-5-3-2-4-6-10/h2-6,9,12H,7-8H2,1H3
InchiKey: XEVZDIFTSGPTLK-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC(O)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-114.03	kJ/mol	Joback Method
hf	-303.93	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.569		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	623.37	K	Joback Method
tc	824.68	K	Joback Method
tf	335.90	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.03	J/mol×K	623.37	Joback Method
cpg	388.31	J/mol×K	656.92	Joback Method
cpg	399.83	J/mol×K	690.47	Joback Method
cpg	410.64	J/mol×K	724.02	Joback Method
cpg	420.77	J/mol×K	757.57	Joback Method
cpg	430.24	J/mol×K	791.13	Joback Method
cpg	439.09	J/mol×K	824.68	Joback Method
dvisc	0.0075832	Pa×s	335.90	Joback Method

dvisc	0.0021568	Pa×s	383.81	Joback Method
dvisc	0.0008109	Pa×s	431.72	Joback Method
dvisc	0.0003707	Pa×s	479.63	Joback Method
dvisc	0.0001953	Pa×s	527.55	Joback Method
dvisc	0.0001145	Pa×s	575.46	Joback Method
dvisc	0.0000729	Pa×s	623.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389849&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