1-hydroxy-4-phenyl-2-butanone

Inchi: InChI=1S/C10H12O2/c11-8-10(12)7-6-9-4-2-1-3-5-9/h1-5,11H,6-8H2
InchiKey: RWMGQGIAEZVPKY-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: O=C(CO)CCc1ccccc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-120.01	kJ/mol	Joback Method
hf	-278.01	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.181		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
ripol	2432.00		NIST Webbook
ripol	2432.00		NIST Webbook
tb	600.93	K	Joback Method
tc	801.20	K	Joback Method
tf	339.63	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.65	J/mol×K	600.93	Joback Method
cpg	338.96	J/mol×K	634.31	Joback Method
cpg	349.58	J/mol×K	667.69	Joback Method
cpg	359.54	J/mol×K	701.07	Joback Method
cpg	368.88	J/mol×K	734.44	Joback Method
cpg	377.63	J/mol×K	767.82	Joback Method
cpg	385.80	J/mol×K	801.20	Joback Method
dvisc	0.0059165	Pa×s	339.63	Joback Method

dvisc	0.0019932	Pa×s	383.18	Joback Method
dvisc	0.0008385	Pa×s	426.73	Joback Method
dvisc	0.0004141	Pa×s	470.28	Joback Method
dvisc	0.0002305	Pa×s	513.83	Joback Method
dvisc	0.0001406	Pa×s	557.38	Joback Method
dvisc	0.0000921	Pa×s	600.93	Joback Method

Sources

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=R389730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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