3-hydroxy-1-phenyl-2-butanone

Inchi: InChI=1S/C10H12O2/c1-8(11)10(12)7-9-5-3-2-4-6-9/h2-6,8,11H,7H2,1H3
InchiKey: RFHRXUDEWBOJCW-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(O)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-122.45	kJ/mol	Joback Method
hf	-283.29	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.179		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1351.00		NIST Webbook
tb	600.49	K	Joback Method
tc	804.72	K	Joback Method
tf	324.63	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.11	J/mol×K	600.49	Joback Method
cpg	339.69	J/mol×K	634.53	Joback Method
cpg	350.55	J/mol×K	668.57	Joback Method
cpg	360.71	J/mol×K	702.61	Joback Method
cpg	370.22	J/mol×K	736.64	Joback Method
cpg	379.10	J/mol×K	770.68	Joback Method
cpg	387.38	J/mol×K	804.72	Joback Method
dvisc	0.0090484	Pa×s	324.63	Joback Method
dvisc	0.0025745	Pa×s	370.61	Joback Method

dvisc	0.0009668	Pa×s	416.58	Joback Method
dvisc	0.0004411	Pa×s	462.56	Joback Method
dvisc	0.0002319	Pa×s	508.54	Joback Method
dvisc	0.0001356	Pa×s	554.51	Joback Method
dvisc	0.0000861	Pa×s	600.49	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=R515909&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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