

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.11	J/molxK	600.49	Joback Method
cpg	379.10	J/molxK	770.68	Joback Method
cpg	370.22	J/molxK	736.64	Joback Method
cpg	360.71	J/molxK	702.61	Joback Method
cpg	350.55	J/molxK	668.57	Joback Method
cpg	339.69	J/molxK	634.53	Joback Method
cpg	387.38	J/molxK	804.72	Joback Method
dvisc	0.0000861	Paxs	600.49	Joback Method
dvisc	0.0001356	Paxs	554.51	Joback Method

dvisc	0.0002319	Paxs	508.54	Joback Method
dvisc	0.0004411	Paxs	462.56	Joback Method
dvisc	0.0009668	Paxs	416.58	Joback Method
dvisc	0.0025745	Paxs	370.61	Joback Method
dvisc	0.0090484	Paxs	324.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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