

5-phenyl-3-hydroxy-2-pentanone

Inchi:	InChI=1S/C11H14O2/c1-9(12)11(13)8-7-10-5-3-2-4-6-10/h2-6,11,13H,7-8H2,1H3
InchiKey:	KTOZWAALHAIKAM-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	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2370.00		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/molxK	623.37	Joback Method
cpg	388.31	J/molxK	656.92	Joback Method
cpg	399.83	J/molxK	690.47	Joback Method
cpg	410.64	J/molxK	724.02	Joback Method
cpg	420.77	J/molxK	757.57	Joback Method
cpg	430.24	J/molxK	791.13	Joback Method

cpg	439.09	J/mol×K	824.68	Joback Method
dvisc	0.0075832	Paxs	335.90	Joback Method
dvisc	0.0021568	Paxs	383.81	Joback Method
dvisc	0.0008109	Paxs	431.72	Joback Method
dvisc	0.0003707	Paxs	479.63	Joback Method
dvisc	0.0001953	Paxs	527.55	Joback Method
dvisc	0.0001145	Paxs	575.46	Joback Method
dvisc	0.0000729	Paxs	623.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389710&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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