

4-Hexanone, 2-methyl-2-phenyl

Inchi:	InChI=1S/C13H18O/c1-4-12(14)10-13(2,3)11-8-6-5-7-9-11/h5-9H,4,10H2,1-3H3
InchiKey:	VEZKFOIEZCNFBT-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	CCC(=O)CC(C)(C)c1ccccc1
Mol. weight [g/mol]:	190.28

Physical Properties

Property code	Value	Unit	Source
gf	44.91	kJ/mol	Joback Method
hf	-196.45	kJ/mol	Joback Method
hfus	17.65	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.333		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpola	1405.00		NIST Webbook
ripola	1938.00		NIST Webbook
tb	574.16	K	Joback Method
tc	791.55	K	Joback Method
tf	315.04	K	Joback Method
vc	0.650	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.05	J/molxK	574.16	Joback Method
cpg	494.95	J/molxK	755.32	Joback Method
cpg	482.03	J/molxK	719.09	Joback Method
cpg	468.15	J/molxK	682.86	Joback Method
cpg	453.23	J/molxK	646.62	Joback Method
cpg	437.22	J/molxK	610.39	Joback Method
cpg	506.96	J/molxK	791.55	Joback Method
dvisc	0.0001895	Paxs	574.16	Joback Method

dvisc	0.0002536	Paxs	530.97	Joback Method
dvisc	0.0003572	Paxs	487.79	Joback Method
dvisc	0.0005378	Paxs	444.60	Joback Method
dvisc	0.0008842	Paxs	401.41	Joback Method
dvisc	0.0016388	Paxs	358.23	Joback Method
dvisc	0.0035974	Paxs	315.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409339&Units=SI
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

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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