

1-Phenyl-2-hexanone

Other names:	Benzyl n-butyl ketone 2-Hexanone, 1-phenyl- 1-phenylhexan-2-one
Inchi:	InChI=1S/C12H16O/c1-2-3-9-12(13)10-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3
InchiKey:	DYQAZJQDLPPHNB-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CCCCC(=O)Cc1ccccc1
Mol. weight [g/mol]:	176.25
CAS:	25870-62-6

Physical Properties

Property code	Value	Unit	Source
gf	33.65	kJ/mol	Joback Method
hf	-167.06	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.988		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	554.51	K	Joback Method
tc	762.63	K	Joback Method
tf	301.35	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.41	J/molxK	554.51	Joback Method
cpg	383.97	J/molxK	589.20	Joback Method
cpg	398.61	J/molxK	623.88	Joback Method
cpg	412.38	J/molxK	658.57	Joback Method
cpg	425.31	J/molxK	693.25	Joback Method
cpg	437.43	J/molxK	727.94	Joback Method

cpg	448.79	J/mol×K	762.63	Joback Method
dvisc	0.0030718	Paxs	301.35	Joback Method
dvisc	0.0015239	Paxs	343.54	Joback Method
dvisc	0.0008813	Paxs	385.74	Joback Method
dvisc	0.0005678	Paxs	427.93	Joback Method
dvisc	0.0003958	Paxs	470.12	Joback Method
dvisc	0.0002929	Paxs	512.32	Joback Method
dvisc	0.0002268	Paxs	554.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25870626&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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