

3-Phenylbutyrophenone

Other names:	1,3-Diphenyl-1-butanone 1-Butanone, 1,3-diphenyl-
Inchi:	InChI=1S/C16H16O/c1-13(14-8-4-2-5-9-14)12-16(17)15-10-6-3-7-11-15/h2-11,13H,12H2
InchiKey:	GIVFXLVPKFXTCU-UHFFFAOYSA-N
Formula:	C16H16O
SMILES:	CC(CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	224.30
CAS:	1533-20-6

Physical Properties

Property code	Value	Unit	Source
gf	177.30	kJ/mol	Joback Method
hf	-18.37	kJ/mol	Joback Method
hfus	23.35	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.063		Crippen Method
mvol	190.350	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	672.27	K	Joback Method
tc	913.58	K	Joback Method
tf	357.85	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.92	J/mol×K	672.27	Joback Method
cpg	509.97	J/mol×K	712.49	Joback Method
cpg	525.66	J/mol×K	752.71	Joback Method
cpg	540.07	J/mol×K	792.92	Joback Method
cpg	553.29	J/mol×K	833.14	Joback Method
cpg	565.41	J/mol×K	873.36	Joback Method
cpg	576.50	J/mol×K	913.58	Joback Method

dvisc	0.0024590	Paxs	357.85	Joback Method
dvisc	0.0011342	Paxs	410.25	Joback Method
dvisc	0.0006234	Paxs	462.66	Joback Method
dvisc	0.0003870	Paxs	515.06	Joback Method
dvisc	0.0002624	Paxs	567.46	Joback Method
dvisc	0.0001900	Paxs	619.87	Joback Method
dvisc	0.0001446	Paxs	672.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1533206&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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