BETA-PHENYLPROPIOPHENONE

Other names:	«omega»-Benzyl acetophenone
	Benzylacetophenone
	Dihydrochalcone
	Hydrochalcone
	Hydrocinnamophenone
	Phenethyl phenyl ketone
	Phenyl phenethyl ketone
	Propiophenone, 3-phenyl-
	1-Propanone, 1,3-diphenyl-
	1,3-Diphenyl-1-oxopropane
	1,3-Diphenyl-1-propanone
	1,3-Diphenyl-3-propanone
	2-Phenethyl phenyl ketone
	3-Phenylpropiophenone
	NSC 12245
Inchi:	InChI=1S/C15H14O/c16-15(14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-10H,11-12H2
InchiKey:	QGGZBXOADPVUPN-UHFFFAOYSA-N
Formula:	C15H14O
SMILES:	O=C(CCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	210.28

Physical Properties

Property code	Value	Unit	Source
af	0.5428		Cheméo Relay (1.0)
gf	171.32	kJ/mol	Joback Method
hf	31.54	kJ/mol	Cheméo Relay (1.0)
hfus	24.29	kJ/mol	Joback Method
hvap	89.36	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-3.92		Cheméo Relay (1.0)
logp	3.502		Crippen Method
mcvol	176.260	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1834.40		NIST Webbook
rinpol	1834.40		NIST Webbook
tb	591.37	K	Cheméo Relay (1.0)
tc	853.36	K	Cheméo Relay (1.0)

tf	317.95	K	Cheméo Relay (1.0)
vc	0.652	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.98	J/mol×K	649.83	Joback Method
cpg	457.27	J/mol×K	690.06	Joback Method
cpg	472.25	J/mol×K	730.30	Joback Method
cpg	486.02	J/mol×K	770.53	Joback Method
cpg	498.64	J/mol×K	810.77	Joback Method
cpg	510.20	J/mol×K	851.00	Joback Method
cpg	520.79	J/mol×K	891.24	Joback Method
dvisc	0.0020973	Pa×s	361.58	Joback Method
dvisc	0.0010836	Pa×s	409.62	Joback Method
dvisc	0.0006431	Pa×s	457.66	Joback Method
dvisc	0.0004215	Pa×s	505.70	Joback Method
dvisc	0.0002972	Pa×s	553.75	Joback Method
dvisc	0.0002216	Pa×s	601.79	Joback Method
dvisc	0.0001726	Pa×s	649.83	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1083303&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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