Chalcone

Other names:	2-Propen-1-one, 1,3-diphenyl- «alpha»-Benzylideneacetophenone «beta»-Benzoylstyrene «beta»-Phenylacrylophenone Benzalacetophenone Benzylideneacetophenone Benzylidenacetophenone Chalkone Cinnamophenone Phenyl styryl ketone 1-Phenyl-2-benzoylethylene 1,3-Diphenyl-1-propen-3-one 2-Benzalacetophenone 2-Benzylideneacetophenone 3-Phenylacrylophenone 1,3-Diphenyl-2-propen-1-one Acrylophenone, 3-phenyl- 1-Benzoyl-2-phenylethene 1,3-Diphenylpropenone Phenyl 2-phenylvinyl ketone Styryl phenyl ketone 1-Benzoyl-2-phenylethylene «omega»-Benzylideneacetophenone 1,3-Diphenyl-2-propenone NSC 26612
Inchi:	InChI=1S/C15H12O/c16-15(14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-12H
InchiKey:	DQFBYFPFKXHELB-UHFFFAOYSA-N
Formula:	C15H12O
SMILES:	O=C(C=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	208.26
CAS:	94-41-7

Physical Properties

Property code	Value	Unit	Source
chs	-7626.20	kJ/mol	NIST Webbook
gf	251.54	kJ/mol	Joback Method

hf	124.77	kJ/mol	Joback Method
hfs	-24.00	kJ/mol	NIST Webbook
hfus	24.49	kJ/mol	Joback Method
hvap	60.24	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.583		Crippen Method
mcvol	171.960	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1970.60		NIST Webbook
rinpol	1970.60		NIST Webbook
tb	653.99	K	Joback Method
tc	905.95	K	Joback Method
tf	329.00 ± 4.00	K	NIST Webbook
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.04	J/mol×K	653.99	Joback Method
cpg	434.68	J/mol×K	695.98	Joback Method
cpg	448.96	J/mol×K	737.98	Joback Method
cpg	462.00	J/mol×K	779.97	Joback Method
cpg	473.92	J/mol×K	821.97	Joback Method
cpg	484.83	J/mol×K	863.96	Joback Method
cpg	494.84	J/mol×K	905.95	Joback Method
dvisc	0.0019321	Pa×s	356.50	Joback Method
dvisc	0.0009699	Pa×s	406.08	Joback Method
dvisc	0.0005657	Pa×s	455.66	Joback Method
dvisc	0.0003668	Pa×s	505.25	Joback Method
dvisc	0.0002569	Pa×s	554.83	Joback Method
dvisc	0.0001908	Pa×s	604.41	Joback Method
dvisc	0.0001483	Pa×s	653.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94417&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume