2-Propen-1-one, 1,3-diphenyl-, (E)-

Other names:	trans-Chalcone
	trans-Benzalacetophenone
	(E)-Chalcone
	Phenyl (E)-2-phenylethenyl ketone
	Phenyl trans-styryl ketone
	Benzalacetophenone
Inchi:	InChI=1S/C15H12O/c16-15(14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-12H/b12-11+
InchiKey:	DQFBYFPFKXHELB-VAWYXSNFSA-N
Formula:	C15H12O
SMILES:	O=C(C=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	208.26
CAS:	614-47-1

Physical Properties

Property code	Value	Unit	Source
gf	251.54	kJ/mol	Joback Method
hf	124.77	kJ/mol	Joback Method
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
tb	653.99	K	Joback Method
tc	905.95	K	Joback Method
tf	356.50	K	Joback Method
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	484.83	J/mol×K	863.96	Joback Method
cpg	473.92	J/mol×K	821.97	Joback Method

cpg	462.00	J/mol×K	779.97	Joback Method
cpg	448.96	J/mol×K	737.98	Joback Method
cpg	434.68	J/mol×K	695.98	Joback Method
cpg	494.84	J/mol×K	905.95	Joback Method
dvisc	0.0001483	Pa×s	653.99	Joback Method
dvisc	0.0001908	Pa×s	604.41	Joback Method
dvisc	0.0002569	Pa×s	554.83	Joback Method
dvisc	0.0003668	Pa×s	505.25	Joback Method
dvisc	0.0005657	Pa×s	455.66	Joback Method
dvisc	0.0009699	Pa×s	406.08	Joback Method
dvisc	0.0019321	Pa×s	356.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	481.20	K	3.30	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C614471&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume