«beta»-Phenylpropiolophenone

Other names:	Benzoylphenylacetylene
	Diphenylpropynone
	Phenethynyl phenyl ketone
	Phenyl phenylethynyl ketone
	Phenylbenzoylacetylene
	Propiolophenone, 3-phenyl-
	1-Benzoyl-2-phenylacetylene
	1,3-Diphenylpropynone
	2-Propyn-1-one, 1,3-diphenyl-
	3-Phenylpropiolophenone
	Phenylethynyl phenyl ketone
Inchi:	InChI=1S/C15H10O/c16-15(14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-10H
InchiKey:	YECVQOULKHBGEN-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	O=C(C#Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	206.24
CAS:	7338-94-5

Physical Properties

Property code	Value	Unit	Source
chl	-7486.80	kJ/mol	NIST Webbook
gf	374.12	kJ/mol	Joback Method
hf	279.85	kJ/mol	Joback Method
hfl	155.00 ± 6.00	kJ/mol	NIST Webbook
hfl	-114.00	kJ/mol	NIST Webbook
hfus	27.41	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.921		Crippen Method
mcvol	167.660	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	658.83	K	Joback Method
tc	930.59	K	Joback Method
tf	467.68	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.59	J/mol×K	658.83	Joback Method
cpg	413.07	J/mol×K	704.12	Joback Method
cpg	427.14	J/mol×K	749.42	Joback Method
cpg	439.88	J/mol×K	794.71	Joback Method
cpg	451.42	J/mol×K	840.00	Joback Method
cpg	461.85	J/mol×K	885.29	Joback Method
cpg	471.29	J/mol×K	930.59	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7338945&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume