3-Buten-2-one, 3-methyl-4-phenyl-

Other names: «alpha»-Methylbenzylideneacetone
3-methyl-4-phenyl-3-buten-2-one
Inchi: InChI=1S/C11H12O/c1-9(10(2)12)8-11-6-4-3-5-7-11/h3-8H,1-2H3/b9-8+
InchiKey: BQJFBHBDOAIIGS-CMDGGOBGSA-N
Formula: C11H12O
SMILES: CC(=O)C(C)=Cc1ccccc1
Mol. weight [g/mol]: 160.21
CAS: 1901-26-4

Physical Properties

Property code	Value	Unit	Source
gf	96.90	kJ/mol	Joback Method
hf	-38.99	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.679		Crippen Method
mcvol	139.360	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	535.67	K	Joback Method
tc	761.28	K	Joback Method
tf	271.04	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.02	J/mol×K	535.67	Joback Method
cpg	317.55	J/mol×K	573.27	Joback Method
cpg	331.07	J/mol×K	610.87	Joback Method
cpg	343.65	J/mol×K	648.48	Joback Method
cpg	355.35	J/mol×K	686.08	Joback Method
cpg	366.22	J/mol×K	723.68	Joback Method
cpg	376.33	J/mol×K	761.28	Joback Method

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=C1901264&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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