3-Benzylidene-2,4-pentanedione

Other names:	2,4-Pentanedione, 3-(phenylmethylene)-
	Benzalacetylacetone
	Benzylidene acetylacetone
	1,1-Diacetyl-2-phenylethylene
	2-Acetyl-1-phenyl but-1-en-3-one
	2,4-Pentanedione, 3-benzylidene-
	3-Benzylideneacetylacetone
	(2,2-Diacetylvinyl)benzene
	NSC 35140
	3-(phenylmethylene)pentane-2,4-dione
Inchi:	InChI=1S/C12H12O2/c1-9(13)12(10(2)14)8-11-6-4-3-5-7-11/h3-8H,1-2H3
InchiKey:	NYRGMNMVISROGJ-UHFFFAOYSA-N
Formula:	C12H12O2
SMILES:	CC(=O)C(=Cc1ccccc1)C(C)=O
Mol. weight [g/mol]:	188.22
CAS:	4335-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-23.60	kJ/mol	Joback Method
hf	-172.21	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	58.11	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.248		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	612.42	K	Joback Method
tc	841.51	K	Joback Method
tf	332.24	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.36	J/mol×K	612.42	Joback Method
cpg	380.05	J/mol×K	650.60	Joback Method
cpg	392.76	J/mol×K	688.78	Joback Method
cpg	404.52	J/mol×K	726.96	Joback Method
cpg	415.42	J/mol×K	765.15	Joback Method
cpg	425.51	J/mol×K	803.33	Joback Method
cpg	434.86	J/mol×K	841.51	Joback Method

Sources

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=C4335904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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