Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-3-(phenylmethylene)-

Other names: 2-Bornanone, 3-benzylidene-
Benzylidenecamphor
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one-3-benzylidene
3-Benzylidene-2-bornanone
3-Benzylidenecamphor
1,7,7-trimethyl-3-(phenylmethylene)bicyclo[2.2.1]heptan-2-one
(Z)-3-Benzylidene-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one

Inchi: InChI=1S/C17H20O/c1-16(2)14-9-10-17(16,3)15(18)13(14)11-12-7-5-4-6-8-12/h4-8,11,1

InchiKey: OIQXFRANQVWXJF-QBFSEMIESA-N

Formula: C17H20O

SMILES: CC12CCC(C(=Cc3ccccc3)C1=O)C2(C)C

Mol. weight [g/mol]: 240.34

CAS: 15087-24-8

Physical Properties

Property code	Value	Unit	Source
gf	218.25	kJ/mol	Joback Method
hf	-69.77	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	58.13	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.095		Crippen Method
mcvol	202.180	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1944.70		NIST Webbook
rinpol	1944.70		NIST Webbook
tb	703.06	K	Joback Method
tc	958.55	K	Joback Method
tf	462.27	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	582.30	J/mol×K	703.06	Joback Method
cpg	602.86	J/mol×K	745.64	Joback Method
cpg	622.77	J/mol×K	788.22	Joback Method
cpg	642.41	J/mol×K	830.81	Joback Method
cpg	662.19	J/mol×K	873.39	Joback Method
cpg	682.49	J/mol×K	915.97	Joback Method
cpg	703.69	J/mol×K	958.55	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=C15087248&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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