Ethanone, 1-(2,3-dihydro-1,1,2,3,3,6-hexamethyl-1H-inden-5-y

Other names:	Ketone, 1,1,2,3,3,6-hexamethyl-5-indanyl methyl
	Phantolid
	Phantolide
	5-Acetyl-1,1,2,3,3,6-hexamethylindan
	6-Acetyl-1,1,2,3,3,5-hexamethylindan
	1,1,2,3,3,6-hexamethylindan-5-yl methyl ketone
Inchi:	InChI=1S/C17H24O/c1-10-8-14-15(9-13(10)11(2)18)17(6,7)12(3)16(14,4)5/h8-9,12H,1-7
InchiKey:	VDBHOHJWUDKDRW-UHFFFAOYSA-N
Formula:	C17H24O
SMILES:	CC(=O)c1cc2c(cc1C)C(C)(C)C(C)C2(C)C
Mol. weight [g/mol]:	244.37
CAS:	15323-35-0

Physical Properties

Property code	Value	Unit	Source
gf	81.21	kJ/mol	Joback Method
hf	-242.07	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.403		Crippen Method
mcvol	217.340	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
tb	681.73	K	Joback Method
tc	904.75	K	Joback Method
tf	336.60	K	NIST Webbook
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.83	J/mol×K	681.73	Joback Method
cpg	625.71	J/mol×K	718.90	Joback Method
cpg	643.98	J/mol×K	756.07	Joback Method

cpg	661.87	J/mol×K	793.24	Joback Method
cpg	679.63	J/mol×K	830.41	Joback Method
cpg	697.48	J/mol×K	867.58	Joback Method
cpg	715.66	J/mol×K	904.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.00	K	0.30	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=C15323350&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/60-835-8/Ethanone-1-2-3-dihydro-1-1-2-3-3-6-hexamethyl-1H-inden-5-yl.pdf

Generated by Cheméo on 2024-10-12 02:25:13.198468114 +0000 UTC m=+3280775.835437363.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.