Celestolide

Other names:	Ethanone, 1-[6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-1H-inden-4-yl]-
	4-Acetyl-6-tert-butyl-1,1-dimethyl indan
	1-(6-tert-Butyl-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)ethanone
	Indane, 4-acetyl-1,1-dimethyl-6-(1,1-dimethylethyl)
	6-tert-Butyl-1,1-dimethylindan-4-yl methyl ketone
Inchi:	InChI=1S/C17H24O/c1-11(18)14-9-12(16(2,3)4)10-15-13(14)7-8-17(15,5)6/h9-10H,7-8H2
InchiKey:	IKTHMQYJOWTSJO-UHFFFAOYSA-N
Formula:	C17H24O
SMILES:	CC(=O)c1cc(C(C)(C)C)cc2c1CCC2(C)C
Mol. weight [g/mol]:	244.37
CAS:	13171-00-1

Physical Properties

Property code	Value	Unit	Source
gf	104.96	kJ/mol	Joback Method
hf	-225.38	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.411		Crippen Method
mcvol	217.340	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1705.10		NIST Webbook
rinpol	1706.00		NIST Webbook
ripol	2145.00		NIST Webbook
tb	687.60	K	Joback Method
tc	914.88	K	Joback Method
tf	439.52	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.75	J/mol×K	687.60	Joback Method

cpg	627.34	J/mol×K	725.48	Joback Method
cpg	644.99	J/mol×K	763.36	Joback Method
cpg	661.91	J/mol×K	801.24	Joback Method
cpg	678.27	J/mol×K	839.12	Joback Method
cpg	694.29	J/mol×K	877.00	Joback Method
cpg	710.16	J/mol×K	914.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13171001&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume