1H-Inden-1-one, 2,3-dihydro-3,3,5,6-tetramethyl-

Other names: 3,3,5,6-Tetramethyl-1-indanone
Inchi: InChI=1S/C13H16O/c1-8-5-10-11(6-9(8)2)13(3,4)7-12(10)14/h5-6H,7H2,1-4H3
InchiKey: BXABKFVJTUQBMS-UHFFFAOYSA-N
Formula: C13H16O
SMILES: Cc1cc2c(cc1C)C(C)(C)CC2=O
Mol. weight [g/mol]: 188.27
CAS: 54789-22-9

Physical Properties

Property code	Value	Unit	Source
gf	74.77	kJ/mol	Joback Method
hf	-159.19	kJ/mol	Joback Method
hfus	13.65	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.167		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	613.26	K	Joback Method
tc	850.84	K	Joback Method
tf	410.31	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.36	J/mol×K	613.26	Joback Method
cpg	425.87	J/mol×K	652.86	Joback Method
cpg	441.50	J/mol×K	692.45	Joback Method
cpg	456.39	J/mol×K	732.05	Joback Method
cpg	470.68	J/mol×K	771.65	Joback Method
cpg	484.52	J/mol×K	811.25	Joback Method

cpg	498.04	J/mol×K	850.84	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=C54789229&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