(Z)-2,6-Dimethylocta-2,5,7-trien-4-one

Other names:	(Z)-Tagetenone
	cis-Tagetenone
	cis-Ocimenone
	(Z)-Ocimenone
	Ocimenone Z
	(Z)-Ocymenone (tagetenone)
	(Z)-Ocimenone (cis-ocimenone)
Inchi:	InChI=1S/C10H14O/c1-5-9(4)7-10(11)6-8(2)3/h5-7H,1H2,2-4H3/b9-7-
InchiKey:	XUINKEIPBTYUJP-CLFYSBASSA-N
Formula:	C10H14O
SMILES:	C=CC(C)=CC(=O)C=C(C)C
Mol. weight [g/mol]:	150.22
CAS:	33746-71-3

Physical Properties

Property code	Value	Unit	Source
gf	135.58	kJ/mol	Joback Method
hf	-22.02	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1229.00		NIST Webbook

rinpol	1229.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1231.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	486.83	K	Joback Method
tc	686.94	K	Joback Method
tf	212.55	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.46	J/mol×K	486.83	Joback Method
cpg	304.04	J/mol×K	520.18	Joback Method
cpg	316.83	J/mol×K	553.53	Joback Method
cpg	328.85	J/mol×K	586.88	Joback Method
cpg	340.17	J/mol×K	620.23	Joback Method
cpg	350.82	J/mol×K	653.59	Joback Method
cpg	360.87	J/mol×K	686.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33746713&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