5,7-Octadien-4-one, 2,6-dimethyl-, (E)-

Other names:	trans-Tagetone
	(5E)-2,6-Dimethyl-5,7-octadien-4-one
	(E)-Tagetone
	(E)-2,6-Dimethylocta-5,7-dien-4-one
Inchi:	InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5,7-8H,1,6H2,2-4H3/b9-7-
InchiKey:	RJXKHBTYHGBOKV-CLFYSBASSA-N
Formula:	C10H16O
SMILES:	C=CC(C)=CC(=O)CC(C)C
Mol. weight [g/mol]:	152.23
CAS:	6752-80-3

Physical Properties

Property code	Value	Unit	Source
gf	61.47	kJ/mol	Joback Method
hf	-134.73	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1129.00		NIST Webbook

rinpol	1146.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1149.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	482.35	K	Joback Method
tc	674.03	K	Joback Method
tf	216.59	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.71	J/mol×K	482.35	Joback Method
cpg	321.86	J/mol×K	514.30	Joback Method
cpg	335.28	J/mol×K	546.24	Joback Method
cpg	347.99	J/mol×K	578.19	Joback Method
cpg	360.04	J/mol×K	610.14	Joback Method
cpg	371.44	J/mol×K	642.09	Joback Method
cpg	382.25	J/mol×K	674.03	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=C6752803&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume