7-Octen-4-one, 2,6-dimethyl-

Other names:	2,6-Dimethyloct-7-en-4-one
	Dihydrotagetone
Inchi:	InChI=1S/C10H18O/c1-5-9(4)7-10(11)6-8(2)3/h5,8-9H,1,6-7H2,2-4H3
InchiKey:	VUSBHGLIAQXBSW-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CC(C)CC(=O)CC(C)C
Mol. weight [g/mol]:	154.25
CAS:	1879-00-1

Physical Properties

Property code	Value	Unit	Source
gf	-12.64	kJ/mol	Joback Method
hf	-247.44	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	43.15	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1082.00		NIST Webbook

rinpol	1053.00		NIST Webbook
rinpol	1033.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1319.00		NIST Webbook
tb	477.87	K	Joback Method
tc	661.58	K	Joback Method
tf	220.63	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.68	J/mol×K	477.87	Joback Method
cpg	339.32	J/mol×K	508.49	Joback Method
cpg	353.29	J/mol×K	539.11	Joback Method
cpg	366.62	J/mol×K	569.73	Joback Method
cpg	379.32	J/mol×K	600.35	Joback Method
cpg	391.42	J/mol×K	630.97	Joback Method
cpg	402.93	J/mol×K	661.58	Joback Method
dvisc	0.0096846	Pa×s	220.63	Joback Method
dvisc	0.0031833	Pa×s	263.50	Joback Method
dvisc	0.0014286	Pa×s	306.38	Joback Method
dvisc	0.0007805	Pa×s	349.25	Joback Method
dvisc	0.0004867	Pa×s	392.12	Joback Method
dvisc	0.0003331	Pa×s	435.00	Joback Method
dvisc	0.0002440	Pa×s	477.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1879001&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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