

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 cis-Tagetone Tagetone (Z) (Z)-5,7-Octadien-4-one, 3,6-dimethyl (Z)-Tagetone (Z)-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-VQHVLOKHSA-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
af	0.4120		Cheméo Relay (1.0)
hf	-215.21	kJ/mol	Cheméo Relay (1.0)
hfus	17.34	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1134.00		NIST Webbook

rinpol	1134.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1132.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1122.00	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	1149.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1132.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1150.00	NIST Webbook
ripol	1459.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1459.00	NIST Webbook

ripol	1522.00		NIST Webbook
ripol	1501.00		NIST Webbook
tb	432.50	K	Cheméo Relay (1.0)
tc	644.41	K	Cheméo Relay (1.0)
tf	246.60	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3588189&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

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

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