1,7-Octadien-3-one, 2-methyl-6-methylene-

Other names:	2,6-Dimethyleneoct-7-en-3-one
	2-Methyl-6-methyleneocta-1,7-dien-3-one
	2-Methyl-6-methylen-octa-1,7-dien-3-one
	2-Methyl-6-methylene-1,7-octadien-3-one
Inchi:	InChI=1S/C10H14O/c1-5-9(4)6-7-10(11)8(2)3/h5H,1-2,4,6-7H2,3H3
InchiKey:	YZWOKWMEQQCMRN-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	C=CC(=C)CCC(=O)C(=C)C
Mol. weight [g/mol]:	150.22
CAS:	41702-60-7

Physical Properties

Property code	Value	Unit	Source
gf	150.82	kJ/mol	Joback Method
hf	-5.60	kJ/mol	Joback Method
hfus	16.80	kJ/mol	Joback Method
hvap	42.75	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1103.90		NIST Webbook
rinpol	1131.90		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook

tb	471.87	K	Joback Method
tc	661.94	K	Joback Method
tf	219.19	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.52	J/mol×K	471.87	Joback Method
cpg	302.67	J/mol×K	503.55	Joback Method
cpg	315.14	J/mol×K	535.23	Joback Method
cpg	326.96	J/mol×K	566.90	Joback Method
cpg	338.14	J/mol×K	598.58	Joback Method
cpg	348.74	J/mol×K	630.26	Joback Method
cpg	358.76	J/mol×K	661.94	Joback Method

Sources

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=C41702607&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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