3,5,9-Undecatrien-2-one, 6,10-dimethyl-

Other names:	«psi»-Ionone
	Citrylideneacetone
	Pseudoionone
	6,10-Dimethyl-3,5,9-undecatrien-2-one
	2,6-Dimethylundeca-2,6,8-triene-10-one
	2,6-Dimethyl hendeca-2,6,8-trien-10-one
	6,10-dimethylundeca-3,5,9-trien-2-one
Inchi:	InChI=1S/C13H20O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6-7,9-10H,5,8H2,1-4H3
InchiKey:	JXJIQCXXJGRKRJ-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	CC(=O)C=CC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	192.30
CAS:	141-10-6

Physical Properties

Property code	Value	Unit	Source
chl	-7760.50 ± 2.80	kJ/mol	NIST Webbook
chl	-7755.90	kJ/mol	NIST Webbook
gf	153.22	kJ/mol	Joback Method
hf	-92.15	kJ/mol	Joback Method
hfl	-213.40 ± 2.80	kJ/mol	NIST Webbook
hfus	29.01	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1507.90		NIST Webbook
rinpol	1507.90		NIST Webbook
rinpol	1557.60		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1527.00		NIST Webbook

ripol	1976.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2008.00		NIST Webbook
tb	562.95	K	Joback Method
tc	759.70	K	Joback Method
tf	243.04	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.05	J/mol×K	562.95	Joback Method
cpg	445.99	J/mol×K	595.74	Joback Method
cpg	461.03	J/mol×K	628.53	Joback Method
cpg	475.23	J/mol×K	661.33	Joback Method
cpg	488.64	J/mol×K	694.12	Joback Method
cpg	501.32	J/mol×K	726.91	Joback Method
cpg	513.34	J/mol×K	759.70	Joback Method
cpl	382.70	J/mol×K	297.85	NIST Webbook
hvapt	67.60 ± 1.10	kJ/mol	419.50	NIST Webbook

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=C141106&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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