3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (E,E)-

Other names: trans-«psi»-Ionone
trans,trans-Pseudoionone
(E,E)-Pseudoionone
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/b10-6+
InchiKey: JXJIQCXXJGRKRJ-KOOBJXAQSA-N
Formula: C13H20O
SMILES: CC(=O)C=CC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 192.30
CAS: 3548-78-5

Physical Properties

Property code	Value	Unit	Source
chl	-7712.40 ± 3.50	kJ/mol	NIST Webbook
gf	153.22	kJ/mol	Joback Method
hf	-92.15	kJ/mol	Joback Method
hfl	-261.50 ± 3.50	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	1589.40		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1589.40		NIST Webbook
rinpol	1562.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2073.00		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

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=C3548785&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas 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
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