

5,9-Undecadien-2-one, 6,10-dimethyl-

Other names:	6,10-Dimethyl-5,9-undecadien-2-one 6,10-Dimethyl-undeca-5,9-dien-2-one Dihydropseudoionone «alpha», «beta»-Dihydropseudoionone NSC 406679 2,6-Dimethylundeca-2,6-dien-10-one 6,10-Dimethyl-5,9-undecadiene-2-one
Inchi:	InChI=1S/C13H22O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h7,9H,5-6,8,10H2,1-4H3
InchiKey:	HNZUNIKWNYHEJJ-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	CC(=O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	194.31
CAS:	689-67-8

Physical Properties

Property code	Value	Unit	Source
gf	73.00	kJ/mol	Joback Method
hf	-209.37	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.048		Crippen Method
mvol	187.000	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1427.10		NIST Webbook
rinpol	1471.93		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1427.10		NIST Webbook
rinpol	1463.00		NIST Webbook

rinpol	1456.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1427.10		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1451.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1885.00		NIST Webbook
tb	558.79	K	Joback Method
tc	747.57	K	Joback Method
tf	248.12	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.86	J/mol×K	558.79	Joback Method
cpg	465.21	J/mol×K	590.25	Joback Method
cpg	480.72	J/mol×K	621.72	Joback Method
cpg	495.44	J/mol×K	653.18	Joback Method
cpg	509.40	J/mol×K	684.64	Joback Method
cpg	522.65	J/mol×K	716.10	Joback Method
cpg	535.23	J/mol×K	747.57	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C689678&Units=SI>

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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