5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-

Other names:	cis-Geranylacetone
	Nerylacetone
	cis-6,10-dimethyl-5,9-undecadien-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/b12-9-
InchiKey:	HNZUNIKWNYHEJJ-XFXZXTDPSA-N
Formula:	C13H22O
SMILES:	CC(=O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	194.31
CAS:	3879-26-3

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
mcvol	187.000	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1427.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1835.00		NIST Webbook

ripol	1838.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1865.00		NIST Webbook
tb	558.79	K	Joback Method
tc	747.57	K	Joback Method
tf	248.12	K	Joback Method
vc	0.732	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3879263&Units=SI
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

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

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