

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

Other names:	(E)-6,10-Dimethylundeca-5,9-dien-2-one (E)-6,10-dimethyl-5,9- undecadien-2-one (E)-6,10-dimethyl-5,9-undecadien-2-one (E)-Geranylacetone 5,9-Undecadien-2-one, 6,10-dimethyl-, (5E)- 6,10-dimethyl-(E)-5,9-undecadien-2-one 6,10-dimethyl-5,9-undecadien-2-one, (E) Acetone, geranyl- Geranyl acetone Geranylacetone Geranylacetone, trans- trans-Geranylacetone
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-FMIVXFBMSA-N
Formula:	C13H22O
SMILES:	CC(=O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	194.31
CAS:	3796-70-1

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	1448.00		NIST Webbook
rinpol	1444.00		NIST Webbook
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ripol	1856.00		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/molxK	558.79	Joback Method
cpg	465.21	J/molxK	590.25	Joback Method
cpg	480.72	J/molxK	621.72	Joback Method
cpg	495.44	J/molxK	653.18	Joback Method
cpg	509.40	J/molxK	684.64	Joback Method
cpg	522.65	J/molxK	716.10	Joback Method
cpg	535.23	J/molxK	747.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	1.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3796701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Acetylene in Alcohols and Ketones:	https://www.doi.org/10.1021/acs.jced.8b00126
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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