9-Undecen-2-one, 6,10-dimethyl-

Other names:	Citronellylacetone
	3,4,5,6-Tetrahydropseudoionone
	Dihydrogeranylacetone
	6,10-Dimethyl-9-undecen-2-one
	6,10-dimethylundec-9-en-2-one
Inchi:	InChI=1S/C13H24O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h7,12H,5-6,8-10H2,1-4H3
InchiKey:	LGVYUZVANMHKHV-UHFFFAOYSA-N
Formula:	C13H24O
SMILES:	CC(=O)CCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	196.33
CAS:	4433-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-1.11	kJ/mol	Joback Method
hf	-322.08	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.128		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1329.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1329.00		NIST Webbook
tb	554.31	K	Joback Method
tc	736.14	K	Joback Method
tf	252.16	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	467.90	J/mol×K	554.31	Joback Method
cpg	484.75	J/mol×K	584.61	Joback Method
cpg	500.81	J/mol×K	614.92	Joback Method
cpg	516.11	J/mol×K	645.22	Joback Method
cpg	530.67	J/mol×K	675.53	Joback Method
cpg	544.53	J/mol×K	705.83	Joback Method
cpg	557.71	J/mol×K	736.14	Joback Method

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=C4433367&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume