2-Undecanone, 6,10-dimethyl-

Other names:	Hexahydropseudoionone
	Pseudoionone, hexahydro-
	Tetrahydrogeranylacetone
	6,10-Dimethyl-2-undecanone
	6,10-Dimethylundecan-2-one
Inchi:	InChI=1S/C13H26O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h11-12H,5-10H2,1-4H3
InchiKey:	RBGLEUBCAJNCTR-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	CC(=O)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	198.34
CAS:	1604-34-8

Physical Properties

Property code	Value	Unit	Source
chl	-8274.60	kJ/mol	NIST Webbook
gf	-75.22	kJ/mol	Joback Method
hf	-434.79	kJ/mol	Joback Method
hfl	-556.70 ± 9.00	kJ/mol	NIST Webbook
hfus	23.98	kJ/mol	Joback Method
hvap	50.50	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	4.208		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1407.00		NIST Webbook
rinpol	1389.80		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1389.80		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1408.00		NIST Webbook
ripol	1663.00		NIST Webbook

ripol	1660.00		NIST Webbook
ripol	1660.00		NIST Webbook
tb	549.83	K	Joback Method
tc	725.09	K	Joback Method
tf	256.20	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.90	J/mol×K	695.88	Joback Method
cpg	486.63	J/mol×K	549.83	Joback Method
cpg	503.95	J/mol×K	579.04	Joback Method
cpg	520.51	J/mol×K	608.25	Joback Method
cpg	536.34	J/mol×K	637.46	Joback Method
cpg	551.47	J/mol×K	666.67	Joback Method
cpg	579.66	J/mol×K	725.09	Joback Method
cpl	428.40	J/mol×K	313.55	NIST Webbook
dvisc	0.0001875	Pa×s	549.83	Joback Method
dvisc	0.0089844	Pa×s	256.20	Joback Method
dvisc	0.0028107	Pa×s	305.14	Joback Method
dvisc	0.0012124	Pa×s	354.08	Joback Method
dvisc	0.0006414	Pa×s	403.02	Joback Method
dvisc	0.0003895	Pa×s	451.95	Joback Method
dvisc	0.0002608	Pa×s	500.89	Joback Method
hvapt	59.30 ± 0.40	kJ/mol	426.00	NIST Webbook

Sources

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=C1604348&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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