«alpha»-Ionone

Other names:	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-
	«alpha»-Cyclocitrylideneacetone
	(E)-«alpha»-Ionone
	trans-«alpha»-Ionone
	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, trans
	4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, (E)-
	(3E)-4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	«alpha»-(E)-Ionone
	trans-4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (3E)-
	4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one («alpha»-ionone)
	4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
	4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one
Inchi:	InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6-8,12H,5,9H2,1-4H3/b8-7+
InchiKey:	UZFLPKAIBPNNCA-BQYQJAHWSA-N
Formula:	C13H20O
SMILES:	CC(=O)C=CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	192.30
CAS:	127-41-3

Physical Properties

Property code	Value	Unit	Source
gf	41.46	kJ/mol	Joback Method
hf	-211.48	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	51.16	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1408.00		NIST Webbook

rinpol	1434.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1427.00	NIST Webbook
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ripol	1889.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	574.13	K	Joback Method
tc	792.17	K	Joback Method
tf	321.44	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.92	J/mol×K	719.49	Joback Method
cpg	521.90	J/mol×K	755.83	Joback Method
cpg	438.46	J/mol×K	574.13	Joback Method
cpg	457.12	J/mol×K	610.47	Joback Method
cpg	474.66	J/mol×K	646.81	Joback Method
cpg	491.22	J/mol×K	683.15	Joback Method
cpg	536.27	J/mol×K	792.17	Joback Method

hvapt	62.00	kJ/mol	437.50	NIST Webbook
hvapt	67.50	kJ/mol	309.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.20	K	1.70	NIST Webbook

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=C127413&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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