4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-

Other names:	3,4-Dehydro-«beta»-ionone
	Dehydro-«beta»-ionone
	3,4-didehydro-«beta»-ionone
	dehydroionone
Inchi:	InChI=1S/C13H18O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-8H,9H2,1-4H3/b8-7+
InchiKey:	UWWCASOGCPOGJP-BQYQJAHWSA-N
Formula:	C13H18O
SMILES:	CC(=O)C=CC1=C(C)C=CCC1(C)C
Mol. weight [g/mol]:	190.28
CAS:	1203-08-3

Physical Properties

Property code	Value	Unit	Source
gf	69.50	kJ/mol	Joback Method
hf	-144.83	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.434		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1485.30		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1485.30		NIST Webbook
tb	582.94	K	Joback Method
tc	804.13	K	Joback Method
tf	338.96	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.12	J/mol×K	582.94	Joback Method
cpg	433.84	J/mol×K	619.80	Joback Method
cpg	449.57	J/mol×K	656.67	Joback Method
cpg	464.42	J/mol×K	693.53	Joback Method
cpg	478.54	J/mol×K	730.40	Joback Method
cpg	492.06	J/mol×K	767.26	Joback Method
cpg	505.11	J/mol×K	804.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1203083&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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