2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-

Other names: 3-Oxo-«alpha»-ionol
4-(3-Hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one
4-(3-Hydroxybut-1-enyl)-3,5,5-trimethylcyclohex-2-en-1-one

Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-7,10,12,14H,8H2,1-4H3

InchiKey: MDCGEAGEQVMWPE-AATRIKPKSA-N

Formula: C13H20O2

SMILES: CC1=CC(=O)CC(C)(C)C1C=CC(C)O

Mol. weight [g/mol]: 208.30

CAS: 34318-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-91.47	kJ/mol	Joback Method
hf	-394.11	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.485		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1646.90		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1682.00		NIST Webbook
ripol	2623.00		NIST Webbook
ripol	2657.00		NIST Webbook

ripol	2625.00		NIST Webbook
ripol	2677.00		NIST Webbook
ripol	2637.00		NIST Webbook
ripol	2618.00		NIST Webbook
ripol	2644.00		NIST Webbook
ripol	2627.00		NIST Webbook
ripol	2639.00		NIST Webbook
ripol	2627.00		NIST Webbook
ripol	2615.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2637.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2643.00		NIST Webbook
ripol	2637.00		NIST Webbook
ripol	2626.00		NIST Webbook
ripol	2656.00		NIST Webbook
ripol	2625.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2667.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2608.00		NIST Webbook
ripol	2650.00		NIST Webbook
ripol	2608.00		NIST Webbook
tb	679.82	K	Joback Method
tc	891.27	K	Joback Method
tf	385.55	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.02	J/mol×K	679.82	Joback Method
cpg	529.35	J/mol×K	715.06	Joback Method
cpg	544.95	J/mol×K	750.30	Joback Method
cpg	559.91	J/mol×K	785.55	Joback Method
cpg	574.32	J/mol×K	820.79	Joback Method

cpg	588.28	J/mol×K	856.03	Joback Method
cpg	601.88	J/mol×K	891.27	Joback Method

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=C34318213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume