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

Other names: 3-Oxo-7,8-dihydro-«alpha»-ionol
Blumenol C
2-Cyclohexen-1-one, 4-[(3R)-3-hydroxybutyl]-3,5,5-trimethyl-, (4R)-
(9R)-9-Hydroxy-4-megastigmen-3-one
4-(3-hydroxybutyl)-3,5,5-trimethylcyclohex-2-en-1-one

Inchi: InChI=1S/C13H22O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h7,10,12,14H,5-6,8H2,1-4

InchiKey: UEEJDIUOCUCVHN-UHFFFAOYSA-N

Formula: C13H22O2

SMILES: CC1=CC(=O)CC(C)(C)C1CCC(C)O

Mol. weight [g/mol]: 210.31

CAS: 36151-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-171.69	kJ/mol	Joback Method
hf	-511.33	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.709		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1709.70		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1745.00		NIST Webbook
ripol	2704.00		NIST Webbook
ripol	2694.00		NIST Webbook
ripol	2726.00		NIST Webbook
ripol	2730.00		NIST Webbook
ripol	2730.00		NIST Webbook
ripol	2725.00		NIST Webbook
ripol	2732.00		NIST Webbook
ripol	2726.00		NIST Webbook
tb	675.66	K	Joback Method
tc	879.55	K	Joback Method

tf	390.63	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.34	J/mol×K	675.66	Joback Method
cpg	552.14	J/mol×K	709.64	Joback Method
cpg	568.20	J/mol×K	743.62	Joback Method
cpg	583.60	J/mol×K	777.61	Joback Method
cpg	598.42	J/mol×K	811.59	Joback Method
cpg	612.71	J/mol×K	845.57	Joback Method
cpg	626.56	J/mol×K	879.55	Joback Method

Sources

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=C36151027&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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