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

Other names: Dihydro-3-oxo-«beta»-ionol
4-(2,6,6-Trimethyl-3-oxo-cyclohex-1-en-1-yl)but-3-en-2-ol
4-Oxo-7,8-dihydro-«beta»-ionol

Inchi: InChI=1S/C13H22O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h9,14H,5-8H2,1-4H3

InchiKey: KNHUHSLRIKTCIY-UHFFFAOYSA-N

Formula: C13H22O2

SMILES: CC1=C(CCC(C)O)C(C)(C)CCC1=O

Mol. weight [g/mol]: 210.31

CAS: 27185-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-173.61	kJ/mol	Joback Method
hf	-502.46	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	65.96	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.853		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
ripol	2711.00		NIST Webbook
ripol	2694.00		NIST Webbook
ripol	2660.00		NIST Webbook
ripol	2694.00		NIST Webbook
ripol	2672.00		NIST Webbook
ripol	2694.00		NIST Webbook
ripol	2711.00		NIST Webbook
tb	685.31	K	Joback Method
tc	890.14	K	Joback Method
tf	407.39	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.46	J/mol×K	685.31	Joback Method
cpg	548.71	J/mol×K	719.45	Joback Method
cpg	564.29	J/mol×K	753.59	Joback Method
cpg	579.27	J/mol×K	787.72	Joback Method
cpg	593.72	J/mol×K	821.86	Joback Method
cpg	607.72	J/mol×K	856.00	Joback Method
cpg	621.33	J/mol×K	890.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27185791&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume