3-Buten-2-ol, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (3E)-

Other names: «alpha»-Ionol
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-trans-3-buten-2-ol
alpha-Ionol
4-(2,6,6-Trimethyl-2-cyclohexenyl)-3-buten-2-ol, (3E)-
4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol («alpha»-ionol)
4-(2,6,6-Trimethyl)-2-cyclohexen-1-yl-3-buten-2-ol

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6-8,11-12,14H,5,9H2,1-4H3/

InchiKey: PWDOJWCZWKWKSE-BQYQJAHWSA-N

Formula: C13H22O

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

Mol. weight [g/mol]: 194.31

CAS: 25312-34-9

Physical Properties

Property code	Value	Unit	Source
gf	31.12	kJ/mol	Joback Method
hf	-256.41	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.306		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1392.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1888.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1868.00		NIST Webbook
tb	612.00	K	Joback Method
tc	811.83	K	Joback Method
tf	317.33	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.30	J/mol×K	612.00	Joback Method
cpg	497.17	J/mol×K	645.30	Joback Method
cpg	513.17	J/mol×K	678.61	Joback Method
cpg	528.41	J/mol×K	711.91	Joback Method
cpg	542.99	J/mol×K	745.22	Joback Method
cpg	557.00	J/mol×K	778.52	Joback Method
cpg	570.55	J/mol×K	811.83	Joback Method

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=C25312349&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
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