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

Other names: 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-ol
«beta» Ionol
4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-ol
But-3-en-2-ol, 4-(2,6,6-trimethyl-1-cyclohexenyl)-

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8,11,14H,5-6,9H2,1-4H3/b

InchiKey: CNOPDZWOYFOHGN-BQYQJAHWSA-N

Formula: C13H22O

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

Mol. weight [g/mol]: 194.31

CAS: 22029-76-1

Physical Properties

Property code	Value	Unit	Source
gf	29.20	kJ/mol	Joback Method
hf	-247.54	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.450		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1406.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	621.65	K	Joback Method
tc	822.51	K	Joback Method
tf	334.09	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.42	J/mol×K	621.65	Joback Method
cpg	494.64	J/mol×K	655.13	Joback Method
cpg	510.05	J/mol×K	688.60	Joback Method
cpg	524.77	J/mol×K	722.08	Joback Method
cpg	538.89	J/mol×K	755.56	Joback Method
cpg	552.51	J/mol×K	789.03	Joback Method
cpg	565.75	J/mol×K	822.51	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=C22029761&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