

3-Cyclohexen-1-ol, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-

Other names:	«beta»-Bisabolol
Inchi:	InChI=1S/C15H26O/c1-12(2)6-5-7-14(4)15(16)10-8-13(3)9-11-15/h6,8,14,16H,5,7,9-11H
InchiKey:	WTVHAMTYZJGJLJ-LSDHHAIUSA-N
Formula:	C15H26O
SMILES:	CC(C)=CCCC(C)C1(O)CC=C(C)CC1
Mol. weight [g/mol]:	222.37
CAS:	15352-77-9

Physical Properties

Property code	Value	Unit	Source
gf	47.12	kJ/mol	Joback Method
hf	-287.14	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1674.00		NIST Webbook
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rinpol	1675.00		NIST Webbook
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ripol	2143.00	NIST Webbook
ripol	2140.00	NIST Webbook
ripol	2189.00	NIST Webbook
ripol	2140.00	NIST Webbook
ripol	2162.00	NIST Webbook
ripol	2106.00	NIST Webbook
ripol	2143.00	NIST Webbook
ripol	2170.00	NIST Webbook
ripol	2160.00	NIST Webbook

ripol	2151.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2143.00		NIST Webbook
tb	662.31	K	Joback Method
tc	860.22	K	Joback Method
tf	330.15	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.91	J/mol×K	662.31	Joback Method
cpg	601.50	J/mol×K	695.29	Joback Method
cpg	618.27	J/mol×K	728.28	Joback Method
cpg	634.34	J/mol×K	761.26	Joback Method
cpg	649.80	J/mol×K	794.25	Joback Method
cpg	664.78	J/mol×K	827.23	Joback Method
cpg	679.38	J/mol×K	860.22	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=C15352779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

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