Levomenol

Other names:	3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-«alpha»-(4-methyl-3-pentenyl)-, [S-(R*,R*)]- 5-Hepten-2-ol, 6-methyl-2-(4-methyl-3-cyclohexen-1-yl)-, (-)- 3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-«alpha»-(4-methyl-3-pentenyl)-, (-)- ((-))-6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol «alpha»-(-)-Bisabolol «alpha»-Bisabolol (-)-form [S-(R*,R*)]-«alpha»-Bisabolol [S-(R*,R*)]-«alpha»,4-Dimethyl-«alpha»-(4-methyl-3-pentenyl)cyclohex-3-ene-1-methano Kamillosan 6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol, (-)- 3-Cyclohexene-1-methanol, alpha,4-dimethyl-alpha-(4-methyl-3-pentenyl)-, («alpha»S,1S)- l-«alpha»-Bisabolol «alpha»-Bisabolol, L-
Inchi:	InChI=1S/C15H26O/c1-12(2)6-5-11-15(4,16)14-9-7-13(3)8-10-14/h6-7,14,16H,5,8-11H2,
InchiKey:	RGZSQWQPBWRIAQ-LSDHHAIUSA-N
Formula:	C15H26O
SMILES:	CC(C)=CCCC(C)(O)C1CC=C(C)CC1
Mol. weight [g/mol]:	222.37
CAS:	23089-26-1

Physical Properties

Property code	Value	Unit	Source
gf	57.89	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	65.79	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
ripol	2021.00		NIST Webbook
ripol	2021.00		NIST Webbook
tb	659.28	K	Joback Method
tc	857.10	K	Joback Method
tf	323.67	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.62	J/mol×K	659.28	Joback Method
cpg	607.64	J/mol×K	692.25	Joback Method
cpg	624.61	J/mol×K	725.22	Joback Method
cpg	640.58	J/mol×K	758.19	Joback Method
cpg	655.62	J/mol×K	791.16	Joback Method
cpg	669.79	J/mol×K	824.13	Joback Method
cpg	683.15	J/mol×K	857.10	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=C23089261&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume