(S)-2,2,6-Trimethyl-6-((S)-4-methylcyclohex-3-en-1

Other names:	2H-Pyran-3(4H)-one, dihydro-2,2,6-trimethyl-6-(4-methyl-3-cyclohexen-1-yl)-, [S-(R*,R*)]-
	(-)-«alpha»-Bisabolonoxide
	Bisabolone oxide A
	«alpha»-Bisabolone oxide A
	[S-(R*,R*)]-dihydro-2,2,6-trimethyl-6-(4-methyl-3-cyclohexen-1-yl)-2H-pyran-3(4H)-one
	Bisabolon oxide A
Inchi:	InChI=1S/C15H24O2/c1-11-5-7-12(8-6-11)15(4)10-9-13(16)14(2,3)17-15/h5,12H,6-10H2
InchiKey:	MJWZYBQLHJQQJJ-SWLSCSKDSA-N
Formula:	C15H24O2
SMILES:	CC1=CCC(C2(C)CCC(=O)C(C)(C)O2)CC1
Mol. weight [g/mol]:	236.35
CAS:	22567-38-0

Physical Properties

Property code	Value	Unit	Source
gf	-82.75	kJ/mol	Joback Method
hf	-457.54	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.650		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
ripol	2158.00		NIST Webbook
tb	676.42	K	Joback Method
tc	926.73	K	Joback Method
tf	425.20	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.76	J/mol×K	676.42	Joback Method
cpg	623.47	J/mol×K	718.14	Joback Method

cpg	646.11	J/mol×K	759.86	Joback Method
cpg	667.94	J/mol×K	801.58	Joback Method
cpg	689.24	J/mol×K	843.29	Joback Method
cpg	710.26	J/mol×K	885.01	Joback Method
cpg	731.27	J/mol×K	926.73	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=C22567380&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume