2-Furanmethanol, tetrahydro-«alpha»,«alpha»,5-trimethyl-5-(4-methy [2S-[2«alpha»,5«beta»(R*)]]-

Other names:	2-((2S,5S)-5-Methyl-5-((S)-4-methylcyclohex-3-en-1-yl)tetrahydrofuran-2-yl)propan-2-ol
	«alpha»-Bisabolol oxide B
	Bisabolol oxide II
	2-Furanmethanol, tetrahydro-«alpha»,«alpha»,5-trimethyl-5-(4-methyl-3-cyclohexen-1-yl)-
	2-Furanmethanol, tetrahydro-«alpha»,«alpha»,5-trimethyl-5-(4-methyl-3-cyclohexen-1-yl)-, [2S-[2«alpha»,5«beta»(R)]]-
	(-)-Bisabolol oxide B
	(-)-«alpha»-Bisabolol oxide B
	[2S-[2«alpha»,5«beta»(R*)]]-tetrahydro-«alpha»,«alpha»,5-trimethyl-5-(4-methyl-3-cycloh
Inchi:	InChI=1S/C15H26O2/c1-11-5-7-12(8-6-11)15(4)10-9-13(17-15)14(2,3)16/h5,12-13,16H,6
InchiKey:	RKBAYVATPNYHLW-MHEXWIEDSA-N
Formula:	C15H26O2
SMILES:	CC1=CCC(C2(C)CCC(C(C)(C)O)O2)CC1
Mol. weight [g/mol]:	238.37
CAS:	26184-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-76.55	kJ/mol	Joback Method
hf	-489.90	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.441		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1652.00		NIST Webbook

rinpol	1676.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1658.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2163.00		NIST Webbook
tb	693.04	K	Joback Method
tc	909.66	K	Joback Method
tf	399.84	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.37	J/mol×K	693.04	Joback Method
cpg	655.24	J/mol×K	729.14	Joback Method
cpg	674.05	J/mol×K	765.25	Joback Method
cpg	691.94	J/mol×K	801.35	Joback Method
cpg	709.08	J/mol×K	837.46	Joback Method
cpg	725.60	J/mol×K	873.56	Joback Method
cpg	741.67	J/mol×K	909.66	Joback Method

Sources

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=C26184883&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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