(1R,4R)-1-methyl-4-(6-Methylhept-5-en-2-yl)cycloh

Other names: Zingiberenol
Inchi: InChI=1S/C15H26O/c1-12(2)6-5-7-13(3)14-8-10-15(4,16)11-9-14/h6,8,10,13-14,16H,5,7,
InchiKey: VVCHIOKYQRUBED-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)C1C=CC(C)(O)CC1
Mol. weight [g/mol]: 222.37
CAS: 58334-55-7

Physical Properties

Property code	Value	Unit	Source
gf	49.04	kJ/mol	Joback Method
hf	-296.01	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	64.57	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1603.00		NIST Webbook
ripol	2113.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2104.00		NIST Webbook
tb	652.66	K	Joback Method
tc	849.56	K	Joback Method

tf	313.39	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.90	J/mol×K	652.66	Joback Method
cpg	604.08	J/mol×K	685.48	Joback Method
cpg	621.39	J/mol×K	718.29	Joback Method
cpg	637.92	J/mol×K	751.11	Joback Method
cpg	653.79	J/mol×K	783.93	Joback Method
cpg	669.09	J/mol×K	816.75	Joback Method
cpg	683.95	J/mol×K	849.56	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=C58334557&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