Zingiberol

Inchi: InChI=1S/C16H28O/c1-12-6-5-8-16(4)9-7-13(10-14(12)16)11-15(2,3)17/h13-14,17H,1,5-
InchiKey: GMZKBWZWDAAWPI-UHFFFAOYSA-N
Formula: C16H28O
SMILES: C=C1CCCC2(C)CCC(CC(C)(C)O)CC12
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	62.84	kJ/mol	Joback Method
hf	-334.45	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.310		Crippen Method
mcvol	216.150	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1631.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	679.72	K	Joback Method
tc	887.83	K	Joback Method
tf	388.46	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.68	J/mol×K	679.72	Joback Method
cpg	673.06	J/mol×K	714.41	Joback Method
cpg	692.37	J/mol×K	749.09	Joback Method
cpg	710.76	J/mol×K	783.78	Joback Method
cpg	728.38	J/mol×K	818.46	Joback Method
cpg	745.36	J/mol×K	853.15	Joback Method
cpg	761.85	J/mol×K	887.83	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=R558926&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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