

Apofarnesol<(z)-Dihydro->

Other names:	Z-Dihydro-farnesol
Inchi:	InChI=1S/C15H28O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,15-16H,5-6,8,10-12H
InchiKey:	OOOOFOPLSIWRAR-ZROIWOOFSA-N
Formula:	C15H28O
SMILES:	CC(C)=CCCC(C)=CCCC(C)CCO
Mol. weight [g/mol]:	224.38
CAS:	58001-87-9

Physical Properties

Property code	Value	Unit	Source
gf	79.50	kJ/mol	Joback Method
hf	-295.58	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.478		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1576.00		NIST Webbook
tb	642.42	K	Joback Method
tc	816.42	K	Joback Method
tf	266.55	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.29	J/mol×K	642.42	Joback Method
cpg	611.34	J/mol×K	671.42	Joback Method
cpg	626.64	J/mol×K	700.42	Joback Method
cpg	641.24	J/mol×K	729.42	Joback Method

cpg	655.17	J/mol×K	758.42	Joback Method
cpg	668.47	J/mol×K	787.42	Joback Method
cpg	681.19	J/mol×K	816.42	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=C58001879&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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