

Dihydrofarnesol

Other names:	2,3-Dihydrofarnesol (E)-2,3-Dihydrofarnesol 3,7,11-trimethyl-6,10-dodecadien-1-ol
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:	OOOFOPLSIWRAR-NTEUORMPSA-N
Formula:	C15H28O
SMILES:	CC(C)=CCCC(C)=CCCC(C)CCO
Mol. weight [g/mol]:	224.38
CAS:	27745-36-4

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	1677.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1677.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2265.00		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=C27745364&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

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