

2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (E,Z)-

Other names:

(E,Z)-Farnesol
(2E,6Z)-Farnesol
trans,cis-Farnesol
2-trans, 6-cis-Farnesol
Farnesol II (E,Z)

Inchi:

InChI=1S/C15H26O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,11,16H,5-6,8,10,12H

InchiKey:

CRDAMVZIKS XKFV-GNESMGMSA-N

Formula:

C15H26O

SMILES:

CC(C)=CCCC(C)=CCCC(C)=CCO

Mol. weight [g/mol]:

222.37

CAS:

3879-60-5

Physical Properties

Property code	Value	Unit	Source
gf	153.61	kJ/mol	Joback Method
hf	-182.87	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.398		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1695.00		NIST Webbook

rinpol	1696.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1703.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2313.00		NIST Webbook
tb	646.90	K	Joback Method
tc	826.12	K	Joback Method
tf	262.51	K	Joback Method
vc	0.838	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.45	J/mol×K	646.90	Joback Method
cpg	588.94	J/mol×K	676.77	Joback Method
cpg	603.68	J/mol×K	706.64	Joback Method
cpg	617.71	J/mol×K	736.51	Joback Method
cpg	631.10	J/mol×K	766.38	Joback Method
cpg	643.89	J/mol×K	796.25	Joback Method
cpg	656.14	J/mol×K	826.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3879605&Units=SI
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

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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