

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

Other names:

(Z,E)-Farnesol
(2Z,6E)-Farnesol
cis-Farnesol
cis,trans-Farnesol
2-cis,6-trans-Farnesol
(2Z,6E)-3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol
(Z,E)-«alpha»-Farnesol
cis,trans-«alpha»-Farnesol

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: CRDAMVZIKSXKFV-PVMFERMNSA-N

Formula: C15H26O

SMILES: CC(C)=CCCC(C)=CCCC(C)=CCO

Mol. weight [g/mol]: 222.37

CAS: 3790-71-4

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	1661.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1699.00		NIST Webbook

rinpol	1697.00	NIST Webbook
rinpol	1686.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1690.00	NIST Webbook
rinpol	1691.00	NIST Webbook
rinpol	1700.00	NIST Webbook
rinpol	1738.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1678.00	NIST Webbook
rinpol	1673.00	NIST Webbook
rinpol	1654.00	NIST Webbook
rinpol	1696.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1685.00	NIST Webbook
rinpol	1695.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1658.00	NIST Webbook
rinpol	1656.00	NIST Webbook
rinpol	1699.00	NIST Webbook
rinpol	1699.00	NIST Webbook
rinpol	1657.00	NIST Webbook
rinpol	1700.00	NIST Webbook
rinpol	1679.00	NIST Webbook
rinpol	1691.00	NIST Webbook
rinpol	1722.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1701.00	NIST Webbook
rinpol	1690.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1690.00	NIST Webbook
rinpol	1678.00	NIST Webbook
rinpol	1679.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1679.00	NIST Webbook
ripol	2355.00	NIST Webbook
ripol	2352.00	NIST Webbook
ripol	2355.00	NIST Webbook
ripol	2350.00	NIST Webbook
ripol	2339.00	NIST Webbook
ripol	2315.00	NIST Webbook
ripol	2286.00	NIST Webbook
ripol	2351.00	NIST Webbook

ripol	2321.00		NIST Webbook
ripol	2291.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2341.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2341.00		NIST Webbook
ripol	2291.00		NIST Webbook
ripol	2303.00		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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3790714&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
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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