2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-

Other names:	(2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol
	3,7,11,-Trimethyldodeca-2,6,10-trien-1-ol
	3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol (farnesol)
	3,7,11-Trimethyl-2,6,10-dodecatrienol
	3,7,11-trimethyl-2,6,10-dodecatrien-1-ol
	3,7,11-trimethyldodeca-2,6,10-trien-1-ol
	FCI 119a
	Farnesyl alcohol
	NSC 60597
	Stirrup-A/WF
	Stirrup-CRW
	Stirrup-H
	Stirrup-HB
	Stirrup-TPW
	Trimethyl-2,6,10-dodecatriene-1-ol
	farnesol
	«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-YFVJMOTDSA-N
Formula:	C15H26O
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CCO
Mol. weight [g/mol]:	222.37
CAS:	4602-84-0

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	1699.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1682.00		NIST Webbook

rinpol	1698.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1740.00	NIST Webbook
rinpol	1698.00	NIST Webbook
rinpol	1698.00	NIST Webbook
rinpol	1698.00	NIST Webbook
rinpol	1676.00	NIST Webbook
rinpol	1664.00	NIST Webbook
rinpol	1680.00	NIST Webbook
rinpol	1654.00	NIST Webbook
rinpol	1699.00	NIST Webbook
rinpol	1747.00	NIST Webbook
rinpol	1740.00	NIST Webbook
rinpol	1652.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1682.00	NIST Webbook
rinpol	1653.00	NIST Webbook
rinpol	1700.00	NIST Webbook
rinpol	1653.00	NIST Webbook
rinpol	1667.00	NIST Webbook
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rinpol	1746.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1658.00	NIST Webbook
rinpol	1693.00	NIST Webbook
rinpol	1740.00	NIST Webbook
rinpol	1678.70	NIST Webbook
rinpol	1703.50	NIST Webbook
rinpol	1682.50	NIST Webbook
rinpol	1655.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1713.00	NIST Webbook
rinpol	1695.00	NIST Webbook
rinpol	1722.00	NIST Webbook
rinpol	1658.00	NIST Webbook
rinpol	1740.00	NIST Webbook

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ripol	2345.00	NIST Webbook

ripol	2356.00		NIST Webbook
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ripol	2364.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2348.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2350.00		NIST Webbook
tb	646.90	K	Joback Method
tc	826.12	K	Joback Method
tf	262.51	K	Joback Method
vc	0.838	m3/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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	0.50	NIST Webbook

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=C4602840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities in Supercritical Carbon Dioxide of (2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trien-1-ol (Farnesol) and (2S)-5,7-Dihydroxy-2-(4-hydroxyphenyl)chroman-4-one (Naringenin):	https://www.doi.org/10.1021/je900957v

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume