

trans-Farnesol

Other names:

2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (E,E)-
(E,E)-Farnesol
(2E,6E)-Farnesol
all-trans-Farnesol
trans,trans-Farnesol
Inhibitor A2
2-trans,6-trans-Farnesol
2,6-di-trans-Farnesol
(2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol
(E)-Farnesol
Farnesol (2E,6E)
Farnesol, (E,E)-
Farnesol, trans, trans
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (2E,6E)-
trans,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-YFVJMOTDSA-N

Formula:

C15H26O

SMILES:

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

Mol. weight [g/mol]:

222.37

CAS:

106-28-5

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	1724.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1690.00		NIST Webbook

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rinpol	1699.00	NIST Webbook
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ripol	2344.00		NIST Webbook
ripol	2366.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106285&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
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

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