

«alpha»-Farnesene

Other names:

1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (E,E)-Farnesene
2,6,10-Trimethyl-2,6,9,11-dodecatetraene, trans-3,7,11-Trimethyl-1,3,6,10-dodecatetraene, (trans,trans)-(3E,6E)-3,7,11-Trimethyldodeca-1,3,6,10-tetraene
«alpha»-E,E-Farnesene
«alpha»-Farnesene, (E,E)-
«alpha»-trans-Farnesene
«alpha»-trans,trans-Farnesene
(3E,6E)- «alpha»-Farnesene
(E,E)-«alpha»-Farnesene
alpha-Farnesene
trans-«alpha»-Farnesene
trans,trans-«alpha»-Farnesene
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (3E,6E)-trans-2,6,10-Trimethyl-2,6,9,11-dodecatetraene
trans-3,7,11-Trimethyl-1,3,6,10-dodecatetraene
(E,E)-Farnesene
E, «alpha»-Farnesene
(E; E)-«alpha»-farnesene
«alpha»-Farnesene, (Z,E)-
E,E-«alpha», «alpha»-farnesene
(E)-3, (E)-6-«alpha»-farnesene
(E,E)-«alpha»-Farnesene
«alpha»-farnesene (E)
2,6,10-trimethyldodeca-2,6,9,11-tetraene

Inchi: InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,9-10,12H,1,7-8,11H2,2-5H3

InchiKey: CXENHBSYCFKJS-VDQVFBMKSA-N

Formula: C15H24

SMILES: C=CC(C)=CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 204.35

CAS: 502-61-4

Physical Properties

Property code	Value	Unit	Source
gf	378.27	kJ/mol	Joback Method

hf	94.79		kJ/mol	Joback Method
hfus	30.00		kJ/mol	Joback Method
hvap	48.43		kJ/mol	Joback Method
log10ws	-5.52			Crippen Method
logp	5.202			Crippen Method
mcvol	205.010		ml/mol	McGowan Method
pc	1672.79		kPa	Joback Method
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ripol	1734.00	NIST Webbook
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ripol	1736.00	NIST Webbook
ripol	1745.00	NIST Webbook
ripol	1730.00	NIST Webbook
ripol	1745.00	NIST Webbook

ripol	1741.00		NIST Webbook
tb	551.40	K	Joback Method
tc	741.98	K	Joback Method
tf	199.93	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.77	J/mol×K	551.40	Joback Method
cpg	501.93	J/mol×K	583.16	Joback Method
cpg	519.09	J/mol×K	614.93	Joback Method
cpg	535.33	J/mol×K	646.69	Joback Method
cpg	550.70	J/mol×K	678.45	Joback Method
cpg	565.26	J/mol×K	710.22	Joback Method
cpg	579.10	J/mol×K	741.98	Joback Method

Sources

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=C502614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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