1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-

Other names: (Z,E)-«alpha»-Farnesene
(3Z,6E)-3,7,11-Trimethyl-1,3,6,10-dodecatetraene
«alpha»-(Z,E)-Farnesene
(3Z,6E)- «alpha»-Farnesene
cis,trans-«alpha»-Farnesene
(Z)-3, (E)-6-«alpha»-Farnesene
(Z,E)-3,7,11-Trimethyl-1,3,6,10-dodecatetraene,
(Z, E)-farnesene
(Z,E)-«alpha»-Farnesen(3,7,11-Trimethyl-1,3,6,10-dodecatetraen)
1,3,6,10-Dodetetraene, 3,7,11-trimethyl-,[Z,E]

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: CXENHBSYCFFKJS-OXYODPPFSA-N

Formula: C15H24

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

Mol. weight [g/mol]: 204.35

CAS: 26560-14-5

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
rinpol	1488.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1496.00		NIST Webbook

rinpol	1488.00	NIST Webbook
rinpol	1497.00	NIST Webbook
rinpol	1497.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1492.00	NIST Webbook
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rinpol	1499.00	NIST Webbook
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ripol	1732.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	551.40	K	Joback Method
tc	741.98	K	Joback Method

tf	199.93	K	Joback Method
vc	0.799	m3/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=C26560145&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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