

(E,Z)-«alpha»-Farnesene

Other names:	(3E,6Z)-«alpha»-Farnesene
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-DZKMRSEMSA-N
Formula:	C15H24
SMILES:	C=CC(C)=CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hf	-7.48	kJ/mol	Cheméo Relay (1.0)
hfus	30.00	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.65		Cheméo Relay (1.0)
logp	5.202		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1492.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	526.53	K	Cheméo Relay (1.0)
tf	224.45	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U293032&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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