

(Z, Z)-farnesene

Inchi:	InChI=1S/C14H22/c1-5-14(4)12-10-8-6-7-9-11-13(2)3/h5-6,8,11-12H,1,7,9-10H2,2-4H3/t
InchiKey:	ODGXJIQONSQPIF-HWXFIQLYSA-N
Formula:	C14H22
SMILES:	C=CC(C)=CCC=CCCC=C(C)C
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	378.40	kJ/mol	Joback Method
hf	125.22	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	46.12	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.811		Crippen Method
mvol	190.920	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
ripol	1770.00		NIST Webbook
tb	528.64	K	Joback Method
tc	718.28	K	Joback Method
tf	202.62	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.36	J/mol×K	528.64	Joback Method
cpg	451.74	J/mol×K	560.25	Joback Method
cpg	468.16	J/mol×K	591.85	Joback Method
cpg	483.68	J/mol×K	623.46	Joback Method
cpg	498.36	J/mol×K	655.07	Joback Method
cpg	512.26	J/mol×K	686.67	Joback Method
cpg	525.44	J/mol×K	718.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R442212&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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