«alpha»-Farnesene isomer

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-UHFFFAOYSA-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
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	1520.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1511.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R508228&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume