

(E)-«alpha»-Bisabolene

Other names:	trans-«alpha»-Bisabolene
Inchi:	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6-8,15H,5,9-11H2,1-4H3/b
InchiKey:	YHBUQBJHSRGZNF-VGOFMYFVSA-N
Formula:	C15H24
SMILES:	<chem>CC(C)=CCC=C(C)C1CC=C(C)CC1</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	263.54	kJ/mol	Joback Method
hf	-37.44	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1537.00		NIST Webbook

ripol	1530.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1768.00		NIST Webbook
tb	574.37	K	Joback Method
tc	785.97	K	Joback Method
tf	241.39	K	Joback Method
vc	0.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.01	J/mol×K	574.37	Joback Method
cpg	516.16	J/mol×K	609.64	Joback Method
cpg	536.07	J/mol×K	644.90	Joback Method
cpg	554.80	J/mol×K	680.17	Joback Method
cpg	572.42	J/mol×K	715.43	Joback Method
cpg	589.00	J/mol×K	750.70	Joback Method
cpg	604.60	J/mol×K	785.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R231819&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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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