

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-KEQVLUGWSA-N
Formula:	C15H24
SMILES:	CC(C)=CCC=C(C)C1CC=C(C)CC1
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	1536.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	574.37	K	Joback Method
tc	785.97	K	Joback Method
tf	241.39	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=R630850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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