

(E)- «beta»-Bisabolene

Inchi:	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8,15H,4-5,7,9-11H2,1-3H
InchiKey:	XZRVRYPILCSYSP-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C(CCC=C(C)C)C1CC=C(C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	23.58	kJ/mol	Joback Method
hvap	65.73	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-5.58		Cheméo Relay (1.0)
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
tb	545.54	K	Cheméo Relay (1.0)
tf	237.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.97	J/mol×K	566.89	Joback Method
cpg	513.94	J/mol×K	601.37	Joback Method
cpg	533.73	J/mol×K	635.84	Joback Method
cpg	552.38	J/mol×K	670.32	Joback Method
cpg	569.95	J/mol×K	704.80	Joback Method
cpg	586.51	J/mol×K	739.28	Joback Method
cpg	602.09	J/mol×K	773.75	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=R399123&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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