

cis-«beta»-Elemene

Inchi:	InChI=1S/C15H26/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,11,13-14H,1,4,8-10H2,2-
InchiKey:	VGLVBDNQOXVDTC-ZNMIVQPWSA-N
Formula:	C15H26
SMILES:	<chem>C=CC1(C)CCC(C(C)C)CC1C(=C)C</chem>
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	243.65	kJ/mol	Joback Method
hf	-88.26	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	46.00	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.827		Crippen Method
mcvol	202.750	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	545.85	K	Joback Method
tc	753.47	K	Joback Method
tf	249.13	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.32	J/molxK	545.85	Joback Method
cpg	532.57	J/molxK	580.45	Joback Method
cpg	554.50	J/molxK	615.06	Joback Method
cpg	575.21	J/molxK	649.66	Joback Method

cpg	594.81	J/mol×K	684.26	Joback Method
cpg	613.43	J/mol×K	718.86	Joback Method
cpg	631.17	J/mol×K	753.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R427793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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