

(Z)-«beta»-Elemene

Other names:	(-)-cis-«beta»-Elemene
Inchi:	InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5
InchiKey:	OPFTUNCRGUEPRZ-ILXRZTDVSA-N
Formula:	C15H24
SMILES:	<chem>C=CC1(C)CCC(C(=C)C)CC1C(=C)C</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	325.38	kJ/mol	Joback Method
hf	32.66	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	542.85	K	Joback Method
tc	754.13	K	Joback Method
tf	248.41	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.78	J/mol×K	542.85	Joback Method
cpg	511.42	J/mol×K	578.06	Joback Method

cpg	532.71	J/mol×K	613.28	Joback Method
cpg	552.77	J/mol×K	648.49	Joback Method
cpg	571.73	J/mol×K	683.70	Joback Method
cpg	589.70	J/mol×K	718.92	Joback Method
cpg	606.82	J/mol×K	754.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303721&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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