

(E)-«beta»-Elemene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

OPFTUNCRGUEPRZ-ZNMIVQPWSA-N

C15H24

C=CC1(C)CCC(C(=C)C)CC1C(=C)C

204.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.82	kJ/mol	Joback Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
rinpol	1387.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1387.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1593.00		NIST Webbook

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

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=R400169&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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