

(+)-«beta»-Isolongibornene

Inchi:	InChI=1S/C15H24/c1-10-11-6-7-12-13(10)14(2,3)8-5-9-15(11,12)4/h11-13H,1,5-9H2,2-4H
InchiKey:	OYBHJKDJMRMSLX-CDKPOLUSA-N
Formula:	C15H24
SMILES:	C=C1C2C3CCC1C3(C)CCCC2(C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	13.20	kJ/mol	Joback Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1440.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.94	J/mol×K	561.66	Joback Method
cpg	525.20	J/mol×K	599.03	Joback Method
cpg	546.85	J/mol×K	636.41	Joback Method
cpg	567.18	J/mol×K	673.78	Joback Method
cpg	586.48	J/mol×K	711.16	Joback Method
cpg	605.02	J/mol×K	748.53	Joback Method
cpg	623.10	J/mol×K	785.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303701&Units=SI
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):

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

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