

Cubeb-11-ene

Inchi:

lnChI=1S/C15H24/c1-9(2)12-6-5-11(4)15-8-7-10(3)13(15)14(12)15/h10-14H,1,5-8H2,2-4

InchiKey:

RRNQKHLQNVWUCD-MGFOKKCUSA-N

Formula:

C15H24

SMILES:

C=C(C)C1CCC(C)C23CCC(C)C2C13

Mol. weight [g/mol]:

204.35

Physical Properties

Property code	Value	Unit	Source
hfus	21.24	kJ/mol	Joback Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1448.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1448.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1626.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.04	J/mol×K	549.88	Joback Method
cpg	524.93		585.62	Joback Method
cpg	547.24	J/mol×K	621.35	Joback Method
cpg	568.12		657.09	Joback Method
cpg	587.78	J/mol×K	692.82	Joback Method
cpg	606.40		728.56	Joback Method
cpg	624.15	J/mol×K	764.29	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R228972&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):

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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