

Cubeb-11-ene

Inchi:	InChI=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-WWEJYDQOSA-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	1448.00		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	J/mol×K	585.62	Joback Method
cpg	547.24	J/mol×K	621.35	Joback Method
cpg	568.12	J/mol×K	657.09	Joback Method
cpg	587.78	J/mol×K	692.82	Joback Method
cpg	606.40	J/mol×K	728.56	Joback Method
cpg	624.15	J/mol×K	764.29	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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R604910&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

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