

«iota»-Gurjunene

Inchi:

InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h9,11-12,14H,5-8H2,1

InchiKey:

SPCXZDDGSGTVAW-UHFFFAOYSA-N

Formula:

C15H24

SMILES:

CC1=C2C(CC1)C(C)CCC1C2C1(C)C

Mol. weight [g/mol]:

204.35

Physical Properties

Property code	Value	Unit	Source
hfus	21.10	kJ/mol	Joback Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.59	J/mol×K	571.38	Joback Method
cpg	528.29	J/mol×K	607.67	Joback Method
cpg	549.58	J/mol×K	643.96	Joback Method
cpg	569.63	J/mol×K	680.24	Joback Method
cpg	588.60	J/mol×K	716.53	Joback Method
cpg	606.66	J/mol×K	752.82	Joback Method
cpg	624.00	J/mol×K	789.11	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R613197&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

Latest version available from:

<https://www.chemeo.com/cid/74-917-2/iota-Gurjunene.pdf>

Generated by Cheméo on 2026-07-21 05:56:40.07188984 +0000 UTC m=+124495.913775229.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.