

trans-«beta»-Caryophyllene

Inchi: InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h6,13-14H,2,5,7-10H2,1,
InchiKey: NPNUFJAVOOONJE-IOMPXFEGSA-N
Formula: C15H24
SMILES: C=C1CCC=C(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	14.82	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1414.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1425.00		NIST Webbook
ripol	1628.00		NIST Webbook
tb	544.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/mol×K	576.30	Joback Method
cpg	525.28	J/mol×K	613.93	Joback Method
cpg	547.37	J/mol×K	651.55	Joback Method
cpg	568.18	J/mol×K	689.18	Joback Method
cpg	587.84	J/mol×K	726.81	Joback Method
cpg	606.51	J/mol×K	764.43	Joback Method
cpg	624.31	J/mol×K	802.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R607508&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
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/71-426-0/trans-beta-Caryophyllene.pdf>

Generated by Cheméo on 2026-07-21 12:39:50.686912314 +0000 UTC m=+148686.528797723.

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