

Caryophylla-4(12),8(13)-diene-5«beta»-ol

Inchi:	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h12-14,16H,1-2,5-9
InchiKey:	CIIOYOPOMGIECX-RUXDESIVSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(CC2(C)C)C(=C)CCC1O
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.99	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Cheméo Relay (1.0)
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1632.00		NIST Webbook
tb	577.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.21	J/mol×K	658.83	Joback Method
cpg	594.89	J/mol×K	693.49	Joback Method
cpg	613.57	J/mol×K	728.16	Joback Method
cpg	631.35	J/mol×K	762.82	Joback Method
cpg	648.34	J/mol×K	797.48	Joback Method
cpg	664.64	J/mol×K	832.14	Joback Method
cpg	680.34	J/mol×K	866.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R618330&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
tb:	Normal Boiling Point Temperature

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