

«beta»-Caryophyllenol

Inchi:	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
InchiKey:	DWUYGFWOANEJRE-JNUUOJQQSA-N
Formula:	C15H24O
SMILES:	C=C1CCC(O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	19.98	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Cheméo Relay (1.0)
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1655.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	578.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.12	J/mol×K	663.81	Joback Method
cpg	595.62	J/mol×K	698.64	Joback Method
cpg	614.14	J/mol×K	733.48	Joback Method
cpg	631.79	J/mol×K	768.31	Joback Method
cpg	648.66	J/mol×K	803.14	Joback Method
cpg	664.87	J/mol×K	837.98	Joback Method
cpg	680.52	J/mol×K	872.81	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R231191&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>

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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