

4,8-«beta»-Epoxy Caryophyllene

Inchi:	InChI=1S/C15H26O/c1-13(2)10-12-11(13)6-9-14(3)7-5-8-15(12,4)16-14/h11-12H,5-10H2
InchiKey:	FMRYSKILCWLXDC-MXYBEHONSA-N
Formula:	C15H26O
SMILES:	CC12CCCC(C)(O1)C1CC(C)(C)C1CC2
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	13.94	kJ/mol	Joback Method
logp	4.160		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
rinpol	1427.00		NIST Webbook
rinpol	1436.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.99	J/mol×K	593.96	Joback Method
cpg	583.21	J/mol×K	633.45	Joback Method
cpg	605.88	J/mol×K	672.93	Joback Method
cpg	627.44	J/mol×K	712.42	Joback Method
cpg	648.34	J/mol×K	751.91	Joback Method
cpg	669.02	J/mol×K	791.40	Joback Method
cpg	689.92	J/mol×K	830.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R414143&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

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