

LONGIPINENE EPOXIDE

Inchi:	InChI=1S/C15H24O/c1-13(2)6-5-7-14(3)9-8-10-15(4,16-10)12(14)11(9)13/h9-12H,5-8H2
InchiKey:	YIUOYFADMDRLEE-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1(C)CCCC2(C)C3CC4OC4(C)C2C31
Mol. weight [g/mol]:	220.36

Physical Properties

Property code	Value	Unit	Source
hfus	19.44	kJ/mol	Joback Method
logp	3.626		Crippen Method
mcpvol	184.640	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.98	J/mol×K	583.22	Joback Method
cpg	563.50	J/mol×K	621.46	Joback Method
cpg	584.43	J/mol×K	659.71	Joback Method
cpg	604.21	J/mol×K	697.95	Joback Method
cpg	623.32	J/mol×K	736.20	Joback Method
cpg	642.20	J/mol×K	774.44	Joback Method
cpg	661.33	J/mol×K	812.69	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C142792936&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/79-208-4/LONGIPINENE-EPOXIDE.pdf>

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