

10-epi-Junenol

Inchi:	InChI=1S/C15H26O/c1-10(2)12-7-9-15(4)8-5-6-11(3)13(15)14(12)16/h10,12-14,16H,3,5-
InchiKey:	MSJJKJCIFIGTJY-PEUVFPKISA-N
Formula:	C15H26O
SMILES:	<chem>C=C1CCCC2(C)CCC(C(C)C)C(O)C12</chem>
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	17.73	kJ/mol	Joback Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1590.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.74	J/mol×K	654.96	Joback Method
cpg	616.91	J/mol×K	688.98	Joback Method
cpg	636.06	J/mol×K	723.01	Joback Method
cpg	654.29	J/mol×K	757.03	Joback Method
cpg	671.72	J/mol×K	791.05	Joback Method
cpg	688.46	J/mol×K	825.08	Joback Method
cpg	704.61	J/mol×K	859.10	Joback Method

Sources

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):	

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R639877&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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