CHLORANTHALACTONE A

Other names: Dehydroshizukanolide
Inchi: InChI=1S/C15H16O2/c1-7-9-4-12(9)15(3)6-13-10(5-11(7)15)8(2)14(16)17-13/h6,9,11-12
InchiKey: OVEQSZKTJIUNHZ-UHFFFAOYSA-N
Formula: C15H16O2
SMILES: C=C1C2CC2C2(C)C=C3OC(=O)C(C)=C3CC12
Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
hfus	26.36	kJ/mol	Joback Method
logp	2.976		Crippen Method
mcvol	173.310	ml/mol	McGowan Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.18	J/mol×K	681.26	Joback Method
cpg	527.18	J/mol×K	721.32	Joback Method
cpg	543.38	J/mol×K	761.38	Joback Method
cpg	559.02	J/mol×K	801.45	Joback Method
cpg	574.32	J/mol×K	841.51	Joback Method
cpg	589.54	J/mol×K	881.57	Joback Method
cpg	604.90	J/mol×K	921.63	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=C66395026&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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