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
CAS: 66395-02-6

Physical Properties

Property code	Value	Unit	Source
gf	176.23	kJ/mol	Joback Method
hf	-156.96	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.976		Crippen Method
mcvol	173.310	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1943.00		NIST Webbook
tb	681.26	K	Joback Method
tc	921.63	K	Joback Method
tf	498.50	K	Joback Method
vc	0.677	m3/kmol	Joback Method

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66395026&Units=SI
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume