

Aristolactone

Inchi:	InChI=1S/C15H22O2/c1-10(2)13-8-7-11(3)5-4-6-12-9-14(13)17-15(12)16/h5,12-14H,1,4,
InchiKey:	QFJWNYLNCNGSX-XKUGNUBLSA-N
Formula:	C15H22O2
SMILES:	<chem>C=C(C)C1CCC(C)=CCCC2CC1OC2=O</chem>
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	7.52	kJ/mol	Joback Method
hf	-372.38	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.631		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
ripol	2633.00		NIST Webbook
ripol	2633.00		NIST Webbook
tb	672.50	K	Joback Method
tc	913.54	K	Joback Method
tf	361.68	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.54	J/molxK	672.50	Joback Method
cpg	606.76	J/molxK	712.67	Joback Method
cpg	628.33	J/molxK	752.85	Joback Method
cpg	648.26	J/molxK	793.02	Joback Method
cpg	666.57	J/molxK	833.19	Joback Method
cpg	683.27	J/molxK	873.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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