

Argentilactone

Inchi:	InChI=1S/C12H18O2/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h6-8,10-11H,2-5,9H2,1H3/b
InchiKey:	DSPGZXFLJQTNDA-VURMDHGXSA-N
Formula:	C12H18O2
SMILES:	CCCCC=CC1CC=CC(=O)O1
Mol. weight [g/mol]:	194.27
CAS:	64543-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.92	kJ/mol	Joback Method
hf	-331.39	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.995		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1666.00		NIST Webbook
ripol	2515.00		NIST Webbook
tb	591.60	K	Joback Method
tc	807.55	K	Joback Method
tf	322.85	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.62	J/molxK	591.60	Joback Method
cpg	449.61	J/molxK	627.59	Joback Method
cpg	466.60	J/molxK	663.58	Joback Method
cpg	482.60	J/molxK	699.57	Joback Method
cpg	497.63	J/molxK	735.56	Joback Method
cpg	511.72	J/molxK	771.55	Joback Method
cpg	524.87	J/molxK	807.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64543313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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