C-14 massoia lactone

Inchi: InChI=1S/C14H24O2/c1-2-3-4-5-6-7-8-10-13-11-9-12-14(15)16-13/h9,12-13H,2-8,10-11H
InchiKey: CRCMEDPBLYDLQH-ZDUSSCGKSA-N
Formula: C14H24O2
SMILES: CCCCCCCCCC1CC=CC(=O)O1
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-87.30	kJ/mol	Joback Method
hf	-489.89	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.999		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2068.00		NIST Webbook
tb	633.20	K	Joback Method
tc	834.24	K	Joback Method
tf	350.47	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.32	J/mol×K	633.20	Joback Method
cpg	575.63	J/mol×K	666.71	Joback Method
cpg	593.92	J/mol×K	700.21	Joback Method
cpg	611.20	J/mol×K	733.72	Joback Method
cpg	627.49	J/mol×K	767.23	Joback Method
cpg	642.79	J/mol×K	800.73	Joback Method
cpg	657.12	J/mol×K	834.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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