«gamma»-dodec-cis-6,cis-9-dienolactone

Other names: cis,cis-«gamma»-6,9-Dodecadienelactone
Inchi: InChI=1S/C12H18O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h3-4,6-7,11H,2,5,8-10H2,1H
InchiKey: YNHBLISDDXOUDQ-CWWKMNTPSA-N
Formula: C12H18O2
SMILES: CCC=CCC=CCC1CCC(=O)O1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	38.44	kJ/mol	Joback Method
hf	-265.79	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.995		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
ripol	2505.00		NIST Webbook
ripol	2505.00		NIST Webbook
tb	592.33	K	Joback Method
tc	808.22	K	Joback Method
tf	320.53	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.90	J/mol×K	592.33	Joback Method
cpg	448.62	J/mol×K	628.31	Joback Method
cpg	465.31	J/mol×K	664.29	Joback Method
cpg	481.03	J/mol×K	700.28	Joback Method
cpg	495.80	J/mol×K	736.26	Joback Method
cpg	509.67	J/mol×K	772.24	Joback Method
cpg	522.69	J/mol×K	808.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume