«gamma»-2-dodecenolactone

Inchi: InChI=1S/C12H20O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h9-11H,2-8H2,1H3
InchiKey: BWXCHUAWFSHXMU-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CCCCCCCCC1C=CC(=O)O1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-92.04	kJ/mol	Joback Method
hf	-442.45	kJ/mol	Joback Method
hfus	29.48	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.219		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
ripol	2428.00		NIST Webbook
ripol	2428.00		NIST Webbook
tb	583.17	K	Joback Method
tc	783.53	K	Joback Method
tf	331.45	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.74	J/mol×K	583.17	Joback Method
cpg	467.21	J/mol×K	616.56	Joback Method
cpg	483.83	J/mol×K	649.96	Joback Method
cpg	499.59	J/mol×K	683.35	Joback Method
cpg	514.51	J/mol×K	716.74	Joback Method
cpg	528.61	J/mol×K	750.14	Joback Method
cpg	541.89	J/mol×K	783.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R320419&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume