(R)-«gamma»-dodecalactone

Inchi: InChI=1S/C12H22O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h11H,2-10H2,1H3/t11-/m1/s
InchiKey: WGPCZPLRVAWXPW-LLVKDONJSA-N
Formula: C12H22O2
SMILES: CCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-122.00	kJ/mol	Joback Method
hf	-500.23	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.443		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1680.00		NIST Webbook
ripol	2380.00		NIST Webbook
tb	584.01	K	Joback Method
tc	782.64	K	Joback Method
tf	330.69	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.94	J/mol×K	584.01	Joback Method
cpg	488.44	J/mol×K	617.11	Joback Method
cpg	506.05	J/mol×K	650.22	Joback Method
cpg	522.78	J/mol×K	683.32	Joback Method
cpg	538.64	J/mol×K	716.43	Joback Method
cpg	553.64	J/mol×K	749.53	Joback Method
cpg	567.79	J/mol×K	782.64	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=R516759&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
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