(R)-«gamma»-decalactone

Inchi: InChI=1S/C10H18O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h9H,2-8H2,1H3/t9-/m1/s1
InchiKey: IFYYFLINQYPWGJ-SECBINFHSA-N
Formula: C10H18O2
SMILES: CCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-138.84	kJ/mol	Joback Method
hf	-458.95	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
ripol	2140.00		NIST Webbook
tb	538.25	K	Joback Method
tc	742.73	K	Joback Method
tf	308.15	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.23	J/mol×K	538.25	Joback Method
cpg	387.45	J/mol×K	572.33	Joback Method
cpg	403.86	J/mol×K	606.41	Joback Method
cpg	419.47	J/mol×K	640.49	Joback Method
cpg	434.30	J/mol×K	674.57	Joback Method
cpg	448.34	J/mol×K	708.65	Joback Method
cpg	461.59	J/mol×K	742.73	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R516744&Units=SI

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