4-hydroxy-(Z)-non-6-enoic acid, lactone

Inchi: InChI=1S/C9H14O2/c1-2-3-4-5-8-6-7-9(10)11-8/h3-4,8H,2,5-7H2,1H3/b4-3-
InchiKey: FPWNJNJVLBJJSN-ARJAWSKDSA-N
Formula: C9H14O2
SMILES: CCC=CCC1CCC(=O)O1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-67.04	kJ/mol	Joback Method
hf	-321.09	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.048		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1323.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	519.53	K	Joback Method
tc	736.94	K	Joback Method
tf	291.80	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.24	J/mol×K	519.53	Joback Method
cpg	321.24	J/mol×K	555.76	Joback Method
cpg	336.41	J/mol×K	592.00	Joback Method
cpg	350.76	J/mol×K	628.23	Joback Method
cpg	364.31	J/mol×K	664.47	Joback Method
cpg	377.09	J/mol×K	700.70	Joback Method
cpg	389.09	J/mol×K	736.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221208&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume