Cyclopentaneacetic acid, 2-(hydroxymethyl)-3-methyl-, «delta»-lactone

Other names: 7-Methylhexahydrocyclopenta[c]pyran-3(1H)-one
Inchi: InChI=1S/C9H14O2/c1-6-2-3-7-4-9(10)11-5-8(6)7/h6-8H,2-5H2,1H3
InchiKey: VGWJUWSHYRJZKH-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC1CCC2CC(=O)OCC12
Mol. weight [g/mol]: 154.21
CAS: 105181-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-106.32	kJ/mol	Joback Method
hf	-392.01	kJ/mol	Joback Method
hfus	17.60	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.596		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	1443.50		NIST Webbook
rinpol	1443.50		NIST Webbook
tb	521.71	K	Joback Method
tc	754.16	K	Joback Method
tf	307.06	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.14	J/mol×K	521.71	Joback Method
cpg	329.18	J/mol×K	560.45	Joback Method
cpg	347.13	J/mol×K	599.19	Joback Method
cpg	364.01	J/mol×K	637.94	Joback Method
cpg	379.85	J/mol×K	676.68	Joback Method
cpg	394.65	J/mol×K	715.42	Joback Method

cpg	408.45	J/mol×K	754.16	Joback Method

Sources

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=C105181382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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