cis-«beta»-Methyloctalactone

Inchi: InChI=1S/C9H16O2/c1-3-4-8-6-5-7(2)9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8+/m0/s1
InchiKey: HPBBFVUDQZEVHN-JGVFFNPUSA-N
Formula: C9H16O2
SMILES: CCCC1CCC(C)C(=O)O1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-167.07	kJ/mol	Joback Method
hf	-464.81	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	514.97	K	Joback Method
tc	730.13	K	Joback Method
tf	289.12	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.10	J/mol×K	514.97	Joback Method
cpg	341.90	J/mol×K	550.83	Joback Method
cpg	358.91	J/mol×K	586.69	Joback Method
cpg	375.12	J/mol×K	622.55	Joback Method
cpg	390.52	J/mol×K	658.41	Joback Method
cpg	405.09	J/mol×K	694.27	Joback Method

cpg	418.83	J/mol×K	730.13	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=R631160&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume