4-(1-hydroxyethyl)-«gamma»-butanolactone

Other names: 4-(1-Hydroxyethyl)-«gamma»-Butyrolactone
Inchi: InChI=1S/C6H10O3/c1-4(7)5-2-6(8)9-3-5/h4-5,7H,2-3H2,1H3
InchiKey: SDQNMZALKPBELF-UHFFFAOYSA-N
Formula: C6H10O3
SMILES: CC(O)C1COC(=O)C1
Mol. weight [g/mol]: 130.14

Physical Properties

Property code	Value	Unit	Source
hfus	13.28	kJ/mol	Joback Method
logp	-0.070		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
ripol	2431.00		NIST Webbook
ripol	2431.00		NIST Webbook
ripol	2431.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.83	J/mol×K	538.47	Joback Method
cpg	253.35	J/mol×K	572.98	Joback Method
cpg	264.32	J/mol×K	607.50	Joback Method
cpg	274.75	J/mol×K	642.01	Joback Method
cpg	284.64	J/mol×K	676.52	Joback Method
cpg	293.97	J/mol×K	711.03	Joback Method
cpg	302.74	J/mol×K	745.55	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R292374&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices