

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	2328.00		NIST Webbook
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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):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R610341&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

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

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