

4-ethoxy-«gamma»-valerolactone

Inchi:	InChI=1S/C7H12O3/c1-3-9-6-4-7(8)10-5(6)2/h5-6H,3-4H2,1-2H3
InchiKey:	CNOBBQALMRHGQE-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CCOC1CC(=O)OC1C
Mol. weight [g/mol]:	144.17

Physical Properties

Property code	Value	Unit	Source
gf	-276.81	kJ/mol	Joback Method
hf	-549.59	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.727		Crippen Method
mcvol	111.940	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	487.36	K	Joback Method
tc	699.13	K	Joback Method
tf	292.33	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.13	J/molxK	487.36	Joback Method
cpg	273.52	J/molxK	522.66	Joback Method
cpg	287.39	J/molxK	557.95	Joback Method
cpg	300.72	J/molxK	593.25	Joback Method
cpg	313.49	J/molxK	628.54	Joback Method
cpg	325.68	J/molxK	663.84	Joback Method
cpg	337.25	J/molxK	699.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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