

5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester

Other names:	«gamma»-Carboethoxy-«gamma»-butyrolactone 4-(Carboethoxy)-«gamma»--butyrolactone NSC 202561
Inchi:	InChI=1S/C7H10O4/c1-2-10-7(9)5-3-4-6(8)11-5/h5H,2-4H2,1H3
InchiKey:	MJQGWRVDIFBMNW-UHFFFAOYSA-N
Formula:	C7H10O4
SMILES:	CCOC(=O)C1CCC(=O)O1
Mol. weight [g/mol]:	158.15
CAS:	1126-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-398.02	kJ/mol	Joback Method
hf	-641.83	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.35	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.255		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
ripol	2168.00		NIST Webbook
tb	545.90	K	Joback Method
tc	767.11	K	Joback Method
tf	346.50	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.48	J/molxK	545.90	Joback Method
cpg	288.68	J/molxK	582.77	Joback Method
cpg	301.27	J/molxK	619.64	Joback Method
cpg	313.22	J/molxK	656.50	Joback Method
cpg	324.51	J/molxK	693.37	Joback Method

cpg	335.12	J/mol×K	730.24	Joback Method
cpg	345.03	J/mol×K	767.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
hvac:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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