3,4-Diethoxy-3-cyclobutene-1,2-dione

Other names:	3-Cyclobutene-1,2-dione, 3,4-diethoxy-
	Diethyl squarate
Inchi:	InChI=1S/C8H10O4/c1-3-11-7-5(9)6(10)8(7)12-4-2/h3-4H2,1-2H3
InchiKey:	DFSFLZCLKYZYRD-UHFFFAOYSA-N
Formula:	C8H10O4
SMILES:	CCOc1c(OCC)c(=O)c1=O
Mol. weight [g/mol]:	170.16
CAS:	5231-87-8

Physical Properties

Property code	Value	Unit	Source
chl	-4025.10 ± 1.40	kJ/mol	NIST Webbook
hf	-478.50 ± 4.10	kJ/mol	NIST Webbook
hfl	-552.10 ± 1.40	kJ/mol	NIST Webbook
hvap	73.60 ± 3.80	kJ/mol	NIST Webbook
log10ws	-0.22		Crippen Method
logp	0.080		Crippen Method
mcvol	123.300	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5231878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation 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