3,4-di-n-Butoxy-3-cyclobutene-1,2-dione

Other names:	Dibutyl squarate
	3,4-Dibutoxy-3-cyclobutene-1,2-dione
Inchi:	InChI=1S/C12H18O4/c1-3-5-7-15-11-9(13)10(14)12(11)16-8-6-4-2/h3-8H2,1-2H3
InchiKey:	XBRWELTXMQSEIN-UHFFFAOYSA-N
Formula:	C12H18O4
SMILES:	CCCCOc1c(OCCCC)c(=O)c1=O
Mol. weight [g/mol]:	226.27
CAS:	2892-62-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	1.640		Crippen Method
mcvol	179.660	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.20	K	0.07	NIST Webbook
tbrp	429.00 ± 2.00	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2892628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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