

3,4-DIBUTOXY-3-CYCLOBUTENE-1,2-DIONE

Other names:	3,4-Dibutoxy-3-cyclobutene-1,2-dione Dibutyl squarate
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

Physical Properties

Property code	Value	Unit	Source
af	0.8127		Cheméo Relay (1.0)
gf	-419.21	kJ/mol	Cheméo Relay (1.0, beta)
hf	-536.50	kJ/mol	Cheméo Relay (1.0)
hvap	77.02	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-3.19		Cheméo Relay (1.0)
logp	1.640		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2021.30	kPa	Cheméo Relay (1.0, beta)
tb	550.84	K	Cheméo Relay (1.0)
tc	757.87	K	Cheméo Relay (1.0)
tf	268.67	K	Cheméo Relay (1.0)
vc	0.706	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2892628&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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