Butopyronoxyl

Other names:	2H-Pyran-6-carboxylic acid, 3,4-dihydro-2,2-dimethyl-4-oxo-, butyl ester
	BMOO
	Indalone
	«alpha»,«alpha»-Dimethyl-«alpha»'-carbobutoxy-dihydro-«gamma»-pyrone
	n-Butyl ester of 3,4-dihydro-2,2-dimethyl-4-oxo-2H-pyran-6-carboxylic acid
	Butyl 3,4-dihydro-2,2-dimethyl-4-oxo-1-2H-pyran-6-carboxylate
	Butyl 3,4-dihydro-2,2-dimethyl-4-oxo-2H-pyran-6-carboxylate
	Butyldimethyldihydro-«gamma»-pyrone carboxylate
	ENT 9
	2-Carbo-n-butoxy-6,6-dimethyl-5,6-dihydro-1,4-pyrone
	2,2-Dimethyl-6-carbobutoxy-2,3-dihydro-4-pyrone
	3,4-Dihydro-2,2-dimethyl-4-oxo-2H-pyran-6-carboxylic acid, n-butyl ester
	Butyl mesityl oxide oxalate
	NSC 404420
	3,4-Dihydro-2,2-dimethyl-4-oxo-2H-pyran-6-carboxylic acid, butyl ester
Inchi:	InChI=1S/C12H18O4/c1-4-5-6-15-11(14)10-7-9(13)8-12(2,3)16-10/h7H,4-6,8H2,1-3H3
InchiKey:	OKIJSNGRQAOIGZ-UHFFFAOYSA-N
Formula:	C12H18O4
SMILES:	CCCCOC(=O)C1=CC(=O)CC(C)(C)O1
Mol. weight [g/mol]:	226.27
CAS:	532-34-3

Physical Properties

Property code	Value	Unit	Source
gf	-353.18	kJ/mol	Joback Method
hf	-689.64	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.982		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	668.95	K	Joback Method
tc	889.10	K	Joback Method
tf	436.51	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.16	J/mol×K	668.95	Joback Method
cpg	513.47	J/mol×K	705.64	Joback Method
cpg	529.02	J/mol×K	742.33	Joback Method
cpg	543.87	J/mol×K	779.02	Joback Method
cpg	558.11	J/mol×K	815.72	Joback Method
cpg	571.79	J/mol×K	852.41	Joback Method
cpg	584.99	J/mol×K	889.10	Joback Method
hvapt	64.70	kJ/mol	396.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C532343&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume