Benzoic acid, 4-[(butoxycarbonyl)oxy]-, 4-ethoxyphenyl ester

Other names: Butyl p-(p-ethoxyphenoxycarbonyl)-phenyl carbonate
Butyl p-(ethoxyphenoxycarbonyl)phenyl carbonate
Butyl p-(p-ethoxyphenyloxycarbonyl)phenyl carbonate
Butyl para-(para-ethoxyphenoxycarbonyl)phenylcarbonate
BEPC
Carbonic acid, butyl ester, ester with p-ethoxyphenyl p-hydroxybenzoate
4-ethoxyphenyl 4-[(butoxycarbonyl)oxy]benzoate

Inchi: InChI=1S/C20H22O6/c1-3-5-14-24-20(22)26-18-8-6-15(7-9-18)19(21)25-17-12-10-16(11

InchiKey: GIJIKFKGLZGENN-UHFFFAOYSA-N

Formula: C20H22O6

SMILES: CCCCOC(=O)Oc1ccc(C(=O)Oc2ccc(OCC)cc2)cc1

Mol. weight [g/mol]: 358.39

CAS: 16494-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-354.76	kJ/mol	Joback Method
hf	-760.05	kJ/mol	Joback Method
hfus	42.81	kJ/mol	Joback Method
hvap	89.12	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.620		Crippen Method
mcvol	271.760	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
tb	917.74	K	Joback Method
tc	1141.32	K	Joback Method
tf	581.82	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.35	J/mol×K	917.74	Joback Method
cpg	882.11	J/mol×K	1104.06	Joback Method

cpg	875.56	J/mol×K	1066.79	Joback Method
cpg	867.50	J/mol×K	1029.53	Joback Method
cpg	857.95	J/mol×K	992.27	Joback Method
cpg	846.90	J/mol×K	955.00	Joback Method
cpg	887.16	J/mol×K	1141.32	Joback Method
dvisc	0.0000321	Pa×s	917.74	Joback Method
dvisc	0.0000401	Pa×s	861.75	Joback Method
dvisc	0.0000516	Pa×s	805.77	Joback Method
dvisc	0.0000691	Pa×s	749.78	Joback Method
dvisc	0.0000968	Pa×s	693.79	Joback Method
dvisc	0.0001441	Pa×s	637.81	Joback Method
dvisc	0.0002313	Pa×s	581.82	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C16494249&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

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