Benzoic acid 4-ethoxy-5-methoxy-2-methoxymethyl-tetrahydro-ester

Inchi: InChI=1S/C17H24O6/c1-4-22-16-8-12(10-19-2)14(9-15(16)20-3)17(18)23-13-6-5-7-21-11

InchiKey: ZOBJKVPYWJIBMW-UHFFFAOYSA-N

Formula: C17H24O6

SMILES: CCOc1cc(COC)c(C(=O)OC2CCCOC2)cc1OC

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-434.81	kJ/mol	Joback Method
hf	-911.23	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.576		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2060.25		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	820.03	K	Joback Method
tc	1037.10	K	Joback Method
tf	518.13	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.63	J/mol×K	820.03	Joback Method
cpg	785.18	J/mol×K	856.21	Joback Method
cpg	800.27	J/mol×K	892.39	Joback Method
cpg	813.89	J/mol×K	928.57	Joback Method
cpg	826.00	J/mol×K	964.75	Joback Method
cpg	836.59	J/mol×K	1000.93	Joback Method
cpg	845.63	J/mol×K	1037.10	Joback Method
dvisc	0.0003466	Pa×s	518.13	Joback Method

dvisc	0.0002120	Pa×s	568.45	Joback Method
dvisc	0.0001405	Pa×s	618.76	Joback Method
dvisc	0.0000990	Pa×s	669.08	Joback Method
dvisc	0.0000733	Pa×s	719.40	Joback Method
dvisc	0.0000565	Pa×s	769.71	Joback Method
dvisc	0.0000449	Pa×s	820.03	Joback Method

Sources

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=R273744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume