3,4-Diethoxybenzoic acid

Other names: Benzoic acid, 3,4-diethoxy-
Inchi: InChI=1S/C11H14O4/c1-3-14-9-6-5-8(11(12)13)7-10(9)15-4-2/h5-7H,3-4H2,1-2H3,(H,12
InchiKey: VVKCVAPLTRZJHH-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCOc1ccc(C(=O)O)cc1OCC
Mol. weight [g/mol]: 210.23
CAS: 5409-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-340.85	kJ/mol	Joback Method
hf	-586.03	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.182		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	678.61	K	Joback Method
tc	875.09	K	Joback Method
tf	420.40	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.40	J/mol×K	678.61	Joback Method
cpg	473.08	J/mol×K	842.34	Joback Method
cpg	464.20	J/mol×K	809.60	Joback Method
cpg	454.68	J/mol×K	776.85	Joback Method
cpg	444.55	J/mol×K	744.10	Joback Method
cpg	433.78	J/mol×K	711.36	Joback Method
cpg	481.32	J/mol×K	875.09	Joback Method
dvisc	0.0000411	Pa×s	678.61	Joback Method

dvisc	0.0000582	Pa×s	635.58	Joback Method
dvisc	0.0000866	Pa×s	592.54	Joback Method
dvisc	0.0001373	Pa×s	549.50	Joback Method
dvisc	0.0002355	Pa×s	506.47	Joback Method
dvisc	0.0004463	Pa×s	463.44	Joback Method
dvisc	0.0009642	Pa×s	420.40	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=C5409314&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume