3,4-Diethoxybenzaldehyde

Other names: Benzaldehyde, 3,4-diethoxy-
Inchi: InChI=1S/C11H14O3/c1-3-13-10-6-5-9(8-12)7-11(10)14-4-2/h5-8H,3-4H2,1-2H3
InchiKey: SSTRYEXQYQGGAS-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCOc1ccc(C=O)cc1OCC
Mol. weight [g/mol]: 194.23
CAS: 2029-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-174.63	kJ/mol	Joback Method
hf	-406.80	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.296		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
tb	581.22	K	Joback Method
tc	785.64	K	Joback Method
tf	351.65	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.08	J/mol×K	581.22	Joback Method
cpg	384.41	J/mol×K	615.29	Joback Method
cpg	397.10	J/mol×K	649.36	Joback Method
cpg	409.16	J/mol×K	683.43	Joback Method
cpg	420.57	J/mol×K	717.50	Joback Method
cpg	431.34	J/mol×K	751.57	Joback Method
cpg	441.46	J/mol×K	785.64	Joback Method
dvisc	0.0011708	Pa×s	351.65	Joback Method

dvisc	0.0007257	Pa×s	389.91	Joback Method
dvisc	0.0004900	Pa×s	428.17	Joback Method
dvisc	0.0003528	Pa×s	466.44	Joback Method
dvisc	0.0002671	Pa×s	504.70	Joback Method
dvisc	0.0002102	Pa×s	542.96	Joback Method
dvisc	0.0001708	Pa×s	581.22	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=C2029949&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