3,4-DIMETHOXY-5-HYDROXYBENZALDEHYDE

Other names: Benzaldehyde, 3-hydroxy-4,5-dimethoxy-
Inchi: InChI=1S/C9H10O4/c1-12-8-4-6(5-10)3-7(11)9(8)13-2/h3-5,11H,1-2H3
InchiKey: NVLTWXMZECWWPC-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COc1cc(C=O)cc(O)c1OC
Mol. weight [g/mol]: 182.18

Physical Properties

Property code	Value	Unit	Source
hfus	22.78	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.47		Cheméo Relay (1.0)
logp	1.222		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
tb	560.28	K	Cheméo Relay (1.0)
tf	379.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.35	J/mol×K	616.08	Joback Method
cpg	379.60	J/mol×K	837.67	Joback Method
cpg	371.79	J/mol×K	800.74	Joback Method
cpg	363.52	J/mol×K	763.81	Joback Method
cpg	354.78	J/mol×K	726.88	Joback Method
cpg	345.52	J/mol×K	689.94	Joback Method
cpg	335.72	J/mol×K	653.01	Joback Method
dvisc	0.0000871	Pa×s	528.46	Joback Method
dvisc	0.0000294	Pa×s	616.08	Joback Method
dvisc	0.0000407	Pa×s	586.87	Joback Method
dvisc	0.0000584	Pa×s	557.66	Joback Method
dvisc	0.0003979	Pa×s	440.83	Joback Method
dvisc	0.0001362	Pa×s	499.25	Joback Method
dvisc	0.0002252	Pa×s	470.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.70	K	1.60	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29865905&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point