Propanal, 3-(4-hydroxy-3,5-dimethoxyphenyl)

Inchi: InChI=1S/C11H14O4/c1-14-9-6-8(4-3-5-12)7-10(15-2)11(9)13/h5-7,13H,3-4H2,1-2H3
InchiKey: DPEYEJOFAHQWJI-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COc1cc(CCC=O)cc(OC)c1O
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
gf	-329.25	kJ/mol	Joback Method
hf	-584.11	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.541		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	661.84	K	Joback Method
tc	875.91	K	Joback Method
tf	463.37	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.28	J/mol×K	661.84	Joback Method
cpg	433.31	J/mol×K	697.52	Joback Method
cpg	444.69	J/mol×K	733.20	Joback Method
cpg	455.45	J/mol×K	768.88	Joback Method
cpg	465.63	J/mol×K	804.56	Joback Method
cpg	475.26	J/mol×K	840.23	Joback Method
cpg	484.36	J/mol×K	875.91	Joback Method

dvisc	0.0002966	Pa×s	463.37	Joback Method
dvisc	0.0001615	Pa×s	496.45	Joback Method
dvisc	0.0000949	Pa×s	529.53	Joback Method
dvisc	0.0000593	Pa×s	562.61	Joback Method
dvisc	0.0000391	Pa×s	595.68	Joback Method
dvisc	0.0000269	Pa×s	628.76	Joback Method
dvisc	0.0000192	Pa×s	661.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R88532&Units=SI
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

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