Homosyringaldehyde

Other names: 2-(4-hydroxy-3,5-dimethoxyphenyl)acetaldehyde
1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanal (homosyringaldehyde)
Inchi: InChI=1S/C10H12O4/c1-13-8-5-7(3-4-11)6-9(14-2)10(8)12/h4-6,12H,3H2,1-2H3
InchiKey: KPSSHRNLEXOPHK-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: COc1cc(CC=O)cc(OC)c1O
Mol. weight [g/mol]: 196.20

Physical Properties

Property code	Value	Unit	Source
gf	-337.67	kJ/mol	Joback Method
hf	-563.47	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	66.01	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.151		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	638.96	K	Joback Method
tc	856.64	K	Joback Method
tf	452.10	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.53	J/mol×K	638.96	Joback Method
cpg	383.78	J/mol×K	675.24	Joback Method
cpg	394.42	J/mol×K	711.52	Joback Method
cpg	404.48	J/mol×K	747.80	Joback Method
cpg	413.99	J/mol×K	784.08	Joback Method
cpg	422.98	J/mol×K	820.36	Joback Method
cpg	431.48	J/mol×K	856.64	Joback Method
dvisc	0.0003443	Pa×s	452.10	Joback Method

dvisc	0.0001910	Pa×s	483.24	Joback Method
dvisc	0.0001138	Pa×s	514.39	Joback Method
dvisc	0.0000719	Pa×s	545.53	Joback Method
dvisc	0.0000478	Pa×s	576.67	Joback Method
dvisc	0.0000331	Pa×s	607.82	Joback Method
dvisc	0.0000238	Pa×s	638.96	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=R254169&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