Propanal, 3-(4-hydroxy-3-methoxyphenyl)

Inchi: InChI=1S/C10H12O3/c1-13-10-7-8(3-2-6-11)4-5-9(10)12/h4-7,12H,2-3H2,1H3
InchiKey: KIEATOGEYUWTSR-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COc1cc(CCC=O)ccc1O
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-223.04	kJ/mol	Joback Method
hf	-419.78	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.532		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	611.56	K	Joback Method
tc	831.01	K	Joback Method
tf	417.35	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.47	J/mol×K	611.56	Joback Method
cpg	362.06	J/mol×K	648.14	Joback Method
cpg	372.93	J/mol×K	684.71	Joback Method
cpg	383.15	J/mol×K	721.29	Joback Method
cpg	392.78	J/mol×K	757.86	Joback Method
cpg	401.86	J/mol×K	794.44	Joback Method
cpg	410.46	J/mol×K	831.01	Joback Method

dvisc	0.0007649	Pa×s	417.35	Joback Method
dvisc	0.0003796	Pa×s	449.72	Joback Method
dvisc	0.0002070	Pa×s	482.09	Joback Method
dvisc	0.0001218	Pa×s	514.45	Joback Method
dvisc	0.0000764	Pa×s	546.82	Joback Method
dvisc	0.0000504	Pa×s	579.19	Joback Method
dvisc	0.0000348	Pa×s	611.56	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=R88546&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume