2-Hydroxy-5-methylisophthalaldehyde

Other names: 1,3-Benzenedicarboxaldehyde, 2-hydroxy-5-methyl-
Inchi: InChI=1S/C9H8O3/c1-6-2-7(4-10)9(12)8(3-6)5-11/h2-5,12H,1H3
InchiKey: ZBOUXALQDLLARY-UHFFFAOYSA-N
Formula: C9H8O3
SMILES: Cc1cc(C=O)c(O)c(C=O)c1
Mol. weight [g/mol]: 164.16
CAS: 7310-95-4

Physical Properties

Property code	Value	Unit	Source
gf	-235.61	kJ/mol	Joback Method
hf	-363.97	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.326		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	619.90	K	Joback Method
tc	849.43	K	Joback Method
tf	438.37	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.37	J/mol×K	619.90	Joback Method
cpg	332.18	J/mol×K	811.18	Joback Method
cpg	325.18	J/mol×K	772.92	Joback Method
cpg	317.76	J/mol×K	734.67	Joback Method
cpg	309.87	J/mol×K	696.41	Joback Method
cpg	301.43	J/mol×K	658.16	Joback Method
cpg	338.84	J/mol×K	849.43	Joback Method
dvisc	0.0000509	Pa×s	619.90	Joback Method

dvisc	0.0000709	Pa×s	589.64	Joback Method
dvisc	0.0001021	Pa×s	559.39	Joback Method
dvisc	0.0001535	Pa×s	529.13	Joback Method
dvisc	0.0002425	Pa×s	498.88	Joback Method
dvisc	0.0004062	Pa×s	468.62	Joback Method
dvisc	0.0007307	Pa×s	438.37	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=C7310954&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