

3,5-Dimethoxy-4-hydroxybenzyl alcohol

Other names:	4-Hydroxy-3,5-dimethoxybenzyl alcohol Benzenemethanol, 4-hydroxy-3,5-dimethoxy-
Inchi:	InChI=1S/C9H12O4/c1-12-7-3-6(5-10)4-8(13-2)9(7)11/h3-4,10-11H,5H2,1-2H3
InchiKey:	LUOAEJWSKPQLJD-UHFFFAOYSA-N
Formula:	C9H12O4
SMILES:	COc1cc(CO)cc(OC)c1O
Mol. weight [g/mol]:	184.19
CAS:	530-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-383.39	kJ/mol	Joback Method
hf	-609.48	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.902		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	659.60	K	Joback Method
tc	863.51	K	Joback Method
tf	459.65	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.79	J/mol×K	659.60	Joback Method
cpg	402.22	J/mol×K	829.52	Joback Method
cpg	394.20	J/mol×K	795.54	Joback Method
cpg	385.77	J/mol×K	761.55	Joback Method
cpg	376.91	J/mol×K	727.57	Joback Method
cpg	367.59	J/mol×K	693.58	Joback Method
cpg	409.85	J/mol×K	863.51	Joback Method

dvisc	0.0000056	Pa×s	659.60	Joback Method
dvisc	0.0000088	Pa×s	626.28	Joback Method
dvisc	0.0000146	Pa×s	592.95	Joback Method
dvisc	0.0000255	Pa×s	559.62	Joback Method
dvisc	0.0000478	Pa×s	526.30	Joback Method
dvisc	0.0000978	Pa×s	492.97	Joback Method
dvisc	0.0002217	Pa×s	459.65	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=C530563&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

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