2,4-Dimethoxybenzyl alcohol

Other names: Benzenemethanol, 2,4-dimethoxy-
Inchi: InChI=1S/C9H12O3/c1-11-8-4-3-7(6-10)9(5-8)12-2/h3-5,10H,6H2,1-2H3
InchiKey: RNKOUSCCPHSCFE-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: COc1ccc(CO)c(OC)c1
Mol. weight [g/mol]: 168.19
CAS: 7314-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-228.77	kJ/mol	Joback Method
hf	-432.17	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.196		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	578.98	K	Joback Method
tc	772.90	K	Joback Method
tf	347.93	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.96	J/mol×K	578.98	Joback Method
cpg	322.78	J/mol×K	611.30	Joback Method
cpg	333.13	J/mol×K	643.62	Joback Method
cpg	343.01	J/mol×K	675.94	Joback Method
cpg	352.41	J/mol×K	708.26	Joback Method
cpg	361.32	J/mol×K	740.58	Joback Method
cpg	369.75	J/mol×K	772.90	Joback Method
dvisc	0.0021561	Pa×s	347.93	Joback Method

dvisc	0.0008995	Pa×s	386.44	Joback Method
dvisc	0.0004397	Pa×s	424.95	Joback Method
dvisc	0.0002420	Pa×s	463.46	Joback Method
dvisc	0.0001460	Pa×s	501.96	Joback Method
dvisc	0.0000947	Pa×s	540.47	Joback Method
dvisc	0.0000650	Pa×s	578.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	1.30	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7314445&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume