

2,5-Dimethoxybenzyl alcohol

Other names:	Benzenemethanol, 2,5-dimethoxy-
Inchi:	InChI=1S/C9H12O3/c1-11-8-3-4-9(12-2)7(5-8)6-10/h3-5,10H,6H2,1-2H3
InchiKey:	WGQMUABRZGUAOS-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	COc1ccc(OC)c(CO)c1
Mol. weight [g/mol]:	168.19
CAS:	33524-31-1

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/molxK	578.98	Joback Method
cpg	322.78	J/molxK	611.30	Joback Method
cpg	333.13	J/molxK	643.62	Joback Method
cpg	343.01	J/molxK	675.94	Joback Method
cpg	352.41	J/molxK	708.26	Joback Method
cpg	361.32	J/molxK	740.58	Joback Method
cpg	369.75	J/molxK	772.90	Joback Method
dvisc	0.0021561	Paxs	347.93	Joback Method

dvisc	0.0008995	Paxs	386.44	Joback Method
dvisc	0.0004397	Paxs	424.95	Joback Method
dvisc	0.0002420	Paxs	463.46	Joback Method
dvisc	0.0001460	Paxs	501.96	Joback Method
dvisc	0.0000947	Paxs	540.47	Joback Method
dvisc	0.0000650	Paxs	578.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	0.10	NIST Webbook

Sources

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=C33524311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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