

Benzenemethanol, 3,4-dimethoxy-

Other names:	Veratryl alcohol 3,4-Dimethoxybenzyl alcohol 3,4-Dimethoxyphenylmethyl alcohol 3,4-Dimethoxybenzenemethanol NSC 6317 (3,4-Dimethoxyphenyl)methanol
Inchi:	InChI=1S/C9H12O3/c1-11-8-4-3-7(6-10)5-9(8)12-2/h3-5,10H,6H2,1-2H3
InchiKey:	OEGPRYNGFWGMMV-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	COc1ccc(CO)cc1OC
Mol. weight [g/mol]:	168.19
CAS:	93-03-8

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
rinpol	1449.00		NIST Webbook
rinpol	1506.20		NIST Webbook
rinpol	1456.30		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1506.20		NIST Webbook
rinpol	1456.30		NIST Webbook
rinpol	1449.00		NIST Webbook
ripol	2669.00		NIST Webbook
ripol	2669.00		NIST Webbook
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	361.32	J/mol×K	740.58	Joback Method
cpg	352.41	J/mol×K	708.26	Joback Method
cpg	343.01	J/mol×K	675.94	Joback Method
cpg	333.13	J/mol×K	643.62	Joback Method
cpg	322.78	J/mol×K	611.30	Joback Method
cpg	369.75	J/mol×K	772.90	Joback Method
dvisc	0.0000650	Pa×s	578.98	Joback Method
dvisc	0.0000947	Pa×s	540.47	Joback Method
dvisc	0.0001460	Pa×s	501.96	Joback Method
dvisc	0.0002420	Pa×s	463.46	Joback Method
dvisc	0.0004397	Pa×s	424.95	Joback Method
dvisc	0.0008995	Pa×s	386.44	Joback Method
dvisc	0.0021561	Pa×s	347.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	569.70	K	97.60	NIST Webbook
tbrp	445.20	K	1.60	NIST Webbook

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=C93038&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
ripol:	Polar retention indices
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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