

3,4-Dimethoxyphenethyl alcohol

Other names:	2-(3,4-Dimethoxyphenyl)ethanol Benzeneethanol, 3,4-dimethoxy- Phenethyl alcohol, 3,4-dimethoxy- 1-(2-Hydroxyethyl)-3,4-dimethoxybenzene 3,4-Dimethoxy-«beta»-phenethyl alcohol 3,4-Dimethoxyphenethanol Ethanol, 2-(3,4-dimethoxyphenyl)
Inchi:	InChI=1S/C10H14O3/c1-12-9-4-3-8(5-6-11)7-10(9)13-2/h3-4,7,11H,5-6H2,1-2H3
InchiKey:	SRQAJMUHZROVHW-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	COc1ccc(CCO)cc1OC
Mol. weight [g/mol]:	182.22
CAS:	7417-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-220.35	kJ/mol	Joback Method
hf	-452.81	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.239		Crippen Method
mvol	145.610	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	601.86	K	Joback Method
tc	793.40	K	Joback Method
tf	359.20	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	358.82	J/molxK	601.86	Joback Method
cpg	370.51	J/molxK	633.78	Joback Method
cpg	381.67	J/molxK	665.71	Joback Method
cpg	392.30	J/molxK	697.63	Joback Method
cpg	402.40	J/molxK	729.56	Joback Method
cpg	411.97	J/molxK	761.48	Joback Method
cpg	421.01	J/molxK	793.40	Joback Method
dvisc	0.0018895	Paxs	359.20	Joback Method
dvisc	0.0007786	Paxs	399.64	Joback Method
dvisc	0.0003776	Paxs	440.09	Joback Method
dvisc	0.0002069	Paxs	480.53	Joback Method
dvisc	0.0001244	Paxs	520.97	Joback Method
dvisc	0.0000805	Paxs	561.42	Joback Method
dvisc	0.0000553	Paxs	601.86	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=C7417212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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