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
mcvol	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

cpg	358.82	J/mol×K	601.86	Joback Method
cpg	370.51	J/mol×K	633.78	Joback Method
cpg	381.67	J/mol×K	665.71	Joback Method
cpg	392.30	J/mol×K	697.63	Joback Method
cpg	402.40	J/mol×K	729.56	Joback Method
cpg	411.97	J/mol×K	761.48	Joback Method
cpg	421.01	J/mol×K	793.40	Joback Method
dvisc	0.0018895	Pa×s	359.20	Joback Method
dvisc	0.0007786	Pa×s	399.64	Joback Method
dvisc	0.0003776	Pa×s	440.09	Joback Method
dvisc	0.0002069	Pa×s	480.53	Joback Method
dvisc	0.0001244	Pa×s	520.97	Joback Method
dvisc	0.0000805	Pa×s	561.42	Joback Method
dvisc	0.0000553	Pa×s	601.86	Joback Method

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=C7417212&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume