

1,1-Dimethoxy-2-phenylpropane

Other names:	Hydratropaldehyde dimethyl acetal Benzene, (2,2-dimethoxy-1-methylethyl)- «alpha»-Methylphenacetaldehyde dimethyl acetal Hydratropic aldehyde dimethyl acetal 2-Phenylpropanal dimethylacetal 2-Phenylpropionaldehyde dimethyl acetal Hydrotropaldehyde dimethyl acetal Hydrotropic aldehyde dimethyl acetal
Inchi:	InChI=1S/C11H16O2/c1-9(11(12-2)13-3)10-7-5-4-6-8-10/h4-9,11H,1-3H3
InchiKey:	UFOUDYPOSJJEDJ-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	COC(OC)C(C)c1ccccc1
Mol. weight [g/mol]:	180.24
CAS:	90-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-60.73	kJ/mol	Joback Method
hf	-308.84	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	46.40	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.409		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	521.72	K	Joback Method
tc	729.31	K	Joback Method
tf	254.61	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.58	J/mol×K	521.72	Joback Method

cpg	424.13	J/mol×K	694.71	Joback Method
cpg	411.18	J/mol×K	660.11	Joback Method
cpg	397.45	J/mol×K	625.51	Joback Method
cpg	382.95	J/mol×K	590.92	Joback Method
cpg	367.67	J/mol×K	556.32	Joback Method
cpg	436.32	J/mol×K	729.31	Joback Method
dvisc	0.0001359	Pa×s	521.72	Joback Method
dvisc	0.0001842	Pa×s	477.20	Joback Method
dvisc	0.0002657	Pa×s	432.68	Joback Method
dvisc	0.0004170	Pa×s	388.17	Joback Method
dvisc	0.0007352	Pa×s	343.65	Joback Method
dvisc	0.0015348	Pa×s	299.13	Joback Method
dvisc	0.0041444	Pa×s	254.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.70	K	1.60	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=C90879&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

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