1,2-Dimethoxy-4-(1,2-dimethoxyethyl)benzene

Inchi: InChI=1S/C12H18O4/c1-13-8-12(16-4)9-5-6-10(14-2)11(7-9)15-3/h5-7,12H,8H2,1-4H3
InchiKey: FBZUMNXNTSNNCG-UHFFFAOYSA-N
Formula: C12H18O4
SMILES: COCC(OC)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	-279.13	kJ/mol	Joback Method
hf	-611.58	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.038		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1634.40		NIST Webbook
tb	599.84	K	Joback Method
tc	798.49	K	Joback Method
tf	350.38	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.37	J/mol×K	599.84	Joback Method
cpg	521.68	J/mol×K	765.38	Joback Method
cpg	509.02	J/mol×K	732.27	Joback Method
cpg	495.64	J/mol×K	699.16	Joback Method
cpg	481.55	J/mol×K	666.06	Joback Method
cpg	466.79	J/mol×K	632.95	Joback Method
cpg	533.58	J/mol×K	798.49	Joback Method
dvisc	0.0000812	Pa×s	599.84	Joback Method
dvisc	0.0001027	Pa×s	558.26	Joback Method

dvisc	0.0001350	Pa×s	516.69	Joback Method
dvisc	0.0001862	Pa×s	475.11	Joback Method
dvisc	0.0002731	Pa×s	433.53	Joback Method
dvisc	0.0004345	Pa×s	391.96	Joback Method
dvisc	0.0007717	Pa×s	350.38	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=U313348&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