Methyl (3,4-dimethoxyphenyl)(methoxy)acetate

Inchi: InChI=1S/C12H16O5/c1-14-9-6-5-8(7-10(9)15-2)11(16-3)12(13)17-4/h5-7,11H,1-4H3
InchiKey: SUBCZXXODUGNAT-UHFFFAOYSA-N
Formula: C12H16O5
SMILES: COC(=O)C(OC)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 240.25

Physical Properties

Property code	Value	Unit	Source
gf	-408.05	kJ/mol	Joback Method
hf	-724.16	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	61.90	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.564		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1749.50		NIST Webbook
tb	653.71	K	Joback Method
tc	859.42	K	Joback Method
tf	400.31	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.65	J/mol×K	653.71	Joback Method
cpg	534.50	J/mol×K	825.14	Joback Method
cpg	523.34	J/mol×K	790.85	Joback Method
cpg	511.34	J/mol×K	756.57	Joback Method
cpg	498.54	J/mol×K	722.28	Joback Method
cpg	484.97	J/mol×K	688.00	Joback Method
cpg	544.80	J/mol×K	859.42	Joback Method
dvisc	0.0000832	Pa×s	653.71	Joback Method
dvisc	0.0001044	Pa×s	611.48	Joback Method

dvisc	0.0001354	Pa×s	569.24	Joback Method
dvisc	0.0001830	Pa×s	527.01	Joback Method
dvisc	0.0002609	Pa×s	484.78	Joback Method
dvisc	0.0003979	Pa×s	442.54	Joback Method
dvisc	0.0006632	Pa×s	400.31	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=U333504&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