2-(4-Acetyl-2,5-dimethoxyphenyl)acetic acid, methyl ester

Other names: 4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (oxo-desamino-COOH), methyl-acetylated

Inchi: InChI=1S/C13H16O5/c1-8(14)10-7-11(16-2)9(5-12(10)17-3)6-13(15)18-4/h5,7H,6H2,1-4

InchiKey: FHFAEWSZJXAPON-UHFFFAOYSA-N

Formula: C13H16O5

SMILES: COC(=O)Cc1cc(OC)c(C(C)=O)cc1OC

Mol. weight [g/mol]: 252.26

Physical Properties

Property code	Value	Unit	Source
gf	-430.74	kJ/mol	Joback Method
hf	-731.35	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.622		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	713.46	K	Joback Method
tc	921.93	K	Joback Method
tf	466.80	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.45	J/mol×K	713.46	Joback Method
cpg	524.84	J/mol×K	748.21	Joback Method
cpg	537.41	J/mol×K	782.95	Joback Method
cpg	549.13	J/mol×K	817.70	Joback Method
cpg	559.98	J/mol×K	852.44	Joback Method
cpg	569.95	J/mol×K	887.19	Joback Method
cpg	579.00	J/mol×K	921.93	Joback Method

dvisc	0.0005577	Pa×s	466.80	Joback Method
dvisc	0.0003761	Pa×s	507.91	Joback Method
dvisc	0.0002690	Pa×s	549.02	Joback Method
dvisc	0.0002016	Pa×s	590.13	Joback Method
dvisc	0.0001569	Pa×s	631.24	Joback Method
dvisc	0.0001259	Pa×s	672.35	Joback Method
dvisc	0.0001036	Pa×s	713.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360350&Units=SI
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

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