2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-M (OH-), diacetylated

Inchi: InChI=1S/C15H20O6/c1-9-13(18-4)8-12(6-7-20-10(2)16)15(19-5)14(9)21-11(3)17/h8H,6-

InchiKey: DBRMWDZIBGQKLT-UHFFFAOYSA-N

Formula: C15H20O6

SMILES: COc1cc(CCOC(C)=O)c(OC)c(OC(C)=O)c1C

Mol. weight [g/mol]: 296.32

Physical Properties

Property code	Value	Unit	Source
gf	-528.53	kJ/mol	Joback Method
hf	-916.32	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	77.04	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.043		Crippen Method
mcvol	225.070	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	786.62	K	Joback Method
tc	990.81	K	Joback Method
tf	524.09	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.26	J/mol×K	786.62	Joback Method
cpg	659.05	J/mol×K	820.65	Joback Method
cpg	671.85	J/mol×K	854.68	Joback Method
cpg	683.63	J/mol×K	888.72	Joback Method
cpg	694.34	J/mol×K	922.75	Joback Method
cpg	703.96	J/mol×K	956.78	Joback Method
cpg	712.45	J/mol×K	990.81	Joback Method
dvisc	0.0003164	Pa×s	524.09	Joback Method

dvisc	0.0002181	Pa×s	567.85	Joback Method
dvisc	0.0001585	Pa×s	611.60	Joback Method
dvisc	0.0001202	Pa×s	655.36	Joback Method
dvisc	0.0000944	Pa×s	699.11	Joback Method
dvisc	0.0000763	Pa×s	742.87	Joback Method
dvisc	0.0000631	Pa×s	786.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438372&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