2-(2,5-Dimethoxy-4-ethylphenyl)ethanol, acetate

Other names: 4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (desamino-HO-), acetylated
Inchi: InChI=1S/C14H20O4/c1-5-11-8-14(17-4)12(9-13(11)16-3)6-7-18-10(2)15/h8-9H,5-7H2,1-
InchiKey: KFQOLOALHKPWDS-UHFFFAOYSA-N
Formula: C14H20O4
SMILES: CCc1cc(OC)c(CCOC(C)=O)cc1OC
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-293.40	kJ/mol	Joback Method
hf	-639.41	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.372		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	682.47	K	Joback Method
tc	881.98	K	Joback Method
tf	428.14	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.11	J/mol×K	682.47	Joback Method
cpg	615.14	J/mol×K	848.73	Joback Method
cpg	603.19	J/mol×K	815.48	Joback Method
cpg	590.39	J/mol×K	782.23	Joback Method
cpg	576.77	J/mol×K	748.97	Joback Method
cpg	562.34	J/mol×K	715.72	Joback Method
cpg	626.23	J/mol×K	881.98	Joback Method

dvisc	0.0000913	Pa×s	682.47	Joback Method
dvisc	0.0001122	Pa×s	640.08	Joback Method
dvisc	0.0001419	Pa×s	597.69	Joback Method
dvisc	0.0001861	Pa×s	555.31	Joback Method
dvisc	0.0002552	Pa×s	512.92	Joback Method
dvisc	0.0003703	Pa×s	470.53	Joback Method
dvisc	0.0005786	Pa×s	428.14	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=U360341&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