2,5-Dimethoxy-4-methyl-«beta»-phenethylamine, acetylated

Inchi: InChI=1S/C13H19NO3/c1-9-7-13(17-4)11(8-12(9)16-3)5-6-14-10(2)15/h7-8H,5-6H2,1-4H
InchiKey: QBCJPXLQCVKYTH-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: COc1cc(CCNC(C)=O)c(OC)cc1C
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-107.43	kJ/mol	Joback Method
hf	-433.08	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.691		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	687.34	K	Joback Method
tc	891.28	K	Joback Method
tf	447.30	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.75	J/mol×K	687.34	Joback Method
cpg	536.36	J/mol×K	721.33	Joback Method
cpg	550.16	J/mol×K	755.32	Joback Method
cpg	563.15	J/mol×K	789.31	Joback Method
cpg	575.32	J/mol×K	823.30	Joback Method
cpg	586.67	J/mol×K	857.29	Joback Method
cpg	597.19	J/mol×K	891.28	Joback Method

Sources

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=R438238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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