2-(2,5-Dimethoxy-4-ethylphenyl)ethylamine, N-acetyl-

Other names: 4-ethyl-2,5-dimethoxy-«beta»-phenethylamine, M, N-acetyl
Inchi: InChI=1S/C14H21NO3/c1-5-11-8-14(18-4)12(9-13(11)17-3)6-7-15-10(2)16/h8-9H,5-7H2,
InchiKey: KHPRVOGEBSQNRB-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CCc1cc(OC)c(CCNC(C)=O)cc1OC
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
gf	-99.01	kJ/mol	Joback Method
hf	-453.72	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.945		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	710.22	K	Joback Method
tc	911.83	K	Joback Method
tf	458.57	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.06	J/mol×K	710.22	Joback Method
cpg	590.14	J/mol×K	743.82	Joback Method
cpg	604.36	J/mol×K	777.42	Joback Method
cpg	617.72	J/mol×K	811.02	Joback Method
cpg	630.23	J/mol×K	844.62	Joback Method
cpg	641.87	J/mol×K	878.23	Joback Method
cpg	652.66	J/mol×K	911.83	Joback Method

Sources

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=U360331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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