

2-(2,5-Dimethoxy-4-ethylphenyl)-2-acetoxyethylan

Other names:
N-acetyl-

4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (hydroxyl-N-acetyl)-isomer 3, acetylated

Inchi: CC(=O)OCC1=CC=C(C=C1)C(OC)C(CNC(C)=O)OC(C)=O

InchiKey: QARTUOCHLVMAOF-UHFFFAOYSA-N

Formula: C₁₆H₂₃NO₅

SMILES: CCc1cc(OC)c(C(CNC(C)=O)OC(C)=O)cc1OC

Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
gf	-318.53	kJ/mol	Joback Method
hf	-745.08	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.006		Crippen Method
mcvol	243.270	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	831.83	K	Joback Method
tc	1039.34	K	Joback Method
tf	538.27	K	Joback Method
vc	0.918	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.95	J/molxK	831.83	Joback Method
cpg	744.89	J/molxK	866.41	Joback Method
cpg	757.70	J/molxK	901.00	Joback Method
cpg	769.39	J/molxK	935.58	Joback Method
cpg	779.93	J/molxK	970.17	Joback Method
cpg	789.32	J/molxK	1004.75	Joback Method
cpg	797.55	J/molxK	1039.34	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=U360338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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