

4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (HO-desamino-COOH), isomer 1, methyl-acetylated

SMILES: CCc1cc(OC)c(CC(=O)OC)c(OC(C)=O)c1OC

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	-2.91		Crippen Method
logp	1.907		Crippen Method
mcvol	225.070	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	786.62	K	Joback Method
tc	990.81	K	Joback Method
tf	524.09	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.26	J/molxK	786.62	Joback Method
cpg	703.96	J/molxK	956.78	Joback Method
cpg	694.34	J/molxK	922.75	Joback Method
cpg	683.63	J/molxK	888.72	Joback Method
cpg	671.85	J/molxK	854.68	Joback Method
cpg	659.05	J/molxK	820.65	Joback Method
cpg	712.45	J/molxK	990.81	Joback Method
dvisc	0.0000631	Paxs	786.62	Joback Method
dvisc	0.0000763	Paxs	742.87	Joback Method

dvisc	0.0000944	Paxs	699.11	Joback Method
dvisc	0.0001202	Paxs	655.36	Joback Method
dvisc	0.0001585	Paxs	611.60	Joback Method
dvisc	0.0002181	Paxs	567.85	Joback Method
dvisc	0.0003164	Paxs	524.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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