

2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-N (desamino-HO-), acetylated

InChI: InChI=1S/C13H18O4/c1-7-13(16-11)(8-12(9)15-3)5-6-17-10(2)14/h7-8H,5-6H2,1-4H3
InChIKey: RCHOIQHRDYFARH-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: COc1cc(CCOC(C)=O)c(OC)cc1C
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-301.82	kJ/mol	Joback Method
hf	-618.77	kJ/mol	Joback Method
hfus	27.46	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.118		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	659.59	K	Joback Method
tc	861.54	K	Joback Method
tf	416.87	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.68	J/molxK	659.59	Joback Method
cpg	509.36	J/molxK	693.25	Joback Method
cpg	523.31	J/molxK	726.91	Joback Method
cpg	536.50	J/molxK	760.56	Joback Method
cpg	548.92	J/molxK	794.22	Joback Method
cpg	560.54	J/molxK	827.88	Joback Method
cpg	571.35	J/molxK	861.54	Joback Method
dvisc	0.0006082	Paxs	416.87	Joback Method
dvisc	0.0003956	Paxs	457.32	Joback Method

dvisc	0.0002760	Paxs	497.78	Joback Method
dvisc	0.0002032	Paxs	538.23	Joback Method
dvisc	0.0001562	Paxs	578.68	Joback Method
dvisc	0.0001242	Paxs	619.14	Joback Method
dvisc	0.0001016	Paxs	659.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438258&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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