Propanamide, N-(2,5-dimethoxyphenyl)-2-methyl-

Inchi: InChI=1S/C12H17NO3/c1-8(2)12(14)13-10-7-9(15-3)5-6-11(10)16-4/h5-8H,1-4H3,(H,13,

InchiKey: BSBQTFPDFZGILM-UHFFFAOYSA-N

Formula: C12H17NO3

SMILES: COc1ccc(OC)c(N=C(O)C(C)C)c1

Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
hf	-426.94	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.948		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	723.74	K	Joback Method
tc	930.40	K	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=U307324&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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