1-Adamantanecarboxamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C19H25NO3/c1-22-15-3-4-17(23-2)16(8-15)20-18(21)19-9-12-5-13(10-19)7-14

InchiKey: XIILAZSITCVNCS-UHFFFAOYSA-N

Formula: C19H25NO3

SMILES: COc1ccc(OC)c(N=C(O)C23CC4CC(CC(C4)C2)C3)c1

Mol. weight [g/mol]: 315.41

Physical Properties

Property code	Value	Unit	Source
hf	-359.00	kJ/mol	Joback Method
hvap	84.83	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.508		Crippen Method
mcvol	245.520	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2688.00		NIST Webbook
rinpol	2688.00		NIST Webbook
tb	904.40	K	Joback Method
tc	1134.90	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307470&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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