Carbonic acid, monoamide, N-(3,4-dimethoxyphenethyl)-, 2-methylpropyl ester

Othernames: 3,4-Dimethoxyphenethylamine, N-isoBOC
Inchi: InChI=1S/C15H23NO4/c1-11(2)10-20-15(17)16-8-7-12-5-6-13(18-3)14(9-12)19-4/h5-6,9,
InchiKey: HLGVZYNCZIVZNC-UHFFFAOYSA-N
Formula: C15H23NO4
SMILES: COc1ccc(CCN=C(O)OCC(C)C)cc1OC
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
hf	-621.08	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.833		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	814.80	K	Joback Method
tc	1016.62	K	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=U340209&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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