2,4,5-TRIMETHOXYAMPHETAMINE

Other names:	Phenethylamine, «alpha»-methyl-2,4,5-trimethoxy- TMA-2 2,4,5-Trimethoxy-«alpha»-methylphenethylamine 2,4,5-Trimethoxyamphetamine
Inchi:	InChI=1S/C12H19NO3/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-8H,5,13H2,1-4H3
InchiKey:	TVSIMAWGATVNGK-UHFFFAOYSA-N
Formula:	C12H19NO3
SMILES:	COc1cc(OC)c(OC)cc1CC(C)N
Mol. weight [g/mol]:	225.29

Physical Properties

Property code	Value	Unit	Source
hfus	24.95	kJ/mol	Joback Method
ie	7.71	eV	Cheméo Relay (1.0)
logp	1.602		Crippen Method
mcvol	183.770	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.94	J/mol×K	654.93	Joback Method
cpg	504.12	J/mol×K	689.78	Joback Method
cpg	518.51	J/mol×K	724.63	Joback Method
cpg	532.11	J/mol×K	759.48	Joback Method
cpg	544.90	J/mol×K	794.33	Joback Method
cpg	556.85	J/mol×K	829.17	Joback Method
cpg	567.95	J/mol×K	864.02	Joback Method

Sources

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1083096&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume