Benzeneethanamine, 2,5-dimethoxy-«alpha»,4-dimethyl-

Other names: Phenethylamine, 2,5-dimethoxy-«alpha»,4-dimethyl-
DOM
STP
2,5-Dimethoxy-«alpha»,4-dimethylphenylethylamine
2,5-Dimethoxy-4-methylamphetamine
2,5-Dimethoxy-4-methylphenylisopropylamine
2,5-Dimethoxymethylamphetamine
2',5'-Dimethoxy-4'-methylamphetamine
4-Methyl-2,5-dimethoxyamphetamine
(.+/-.)-1-(2,5-Dimethoxy-4-methylphenyl)-2-aminopropane
(.+/-.)-1-(4-Methyl-2,5-dimethoxyphenyl)-2-aminopropane
(.+/-.)-2,5-Dimethoxy-4-methylamphetamine
(.+/-.)-DOM
(RS)-DOM
dl-2,5-Dimethoxy-4-methylamphetamine
dl-4-Methyl-2,5-dimethoxyamphetamine
STP (hallucinogen)

Inchi: InChI=1S/C12H19NO2/c1-8-5-12(15-4)10(6-9(2)13)7-11(8)14-3/h5,7,9H,6,13H2,1-4H3

InchiKey: NTJQREUGJKIARY-UHFFFAOYSA-N

Formula: C12H19NO2

SMILES: COc1cc(CC(C)N)c(OC)cc1C

Mol. weight [g/mol]: 209.28

CAS: 15588-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-12.31	kJ/mol	Joback Method
hf	-324.82	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	1.902		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1606.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1635.00		NIST Webbook

rinpol	1616.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	632.51	K	Joback Method
tc	843.83	K	Joback Method
tf	401.70	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.71	J/mol×K	632.51	Joback Method
cpg	478.13	J/mol×K	667.73	Joback Method
cpg	492.76	J/mol×K	702.95	Joback Method
cpg	506.60	J/mol×K	738.17	Joback Method
cpg	519.65	J/mol×K	773.39	Joback Method
cpg	531.90	J/mol×K	808.61	Joback Method
cpg	543.34	J/mol×K	843.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15588951&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

cpg: Ideal gas heat capacity
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