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: 26011-50-7

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
ie	7.62 ± 0.06	eV	NIST Webbook
ie	7.62	eV	NIST Webbook
log10ws	-2.95		Crippen Method
logp	1.902		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
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

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=C26011507&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume