Benzeneethanamine, 2,5-dimethoxy-«alpha»-methyl-

Other names: Phenethylamine, 2,5-dimethoxy-«alpha»-methyl-
1-(2,5-Dimethoxyphenyl)-2-aminopropane
2,5-Dimethoxy-«alpha»-methylphenethylamine
2,5-Dimethoxyamphetamine
1-(2,5-Dimethoxyphenyl)-2-propanamine
Amphetamine, 2,5-dimethoxy
DMA

Inchi: InChI=1S/C11H17NO2/c1-8(12)6-9-7-10(13-2)4-5-11(9)14-3/h4-5,7-8H,6,12H2,1-3H3

InchiKey: LATVFYDIBMDBSY-UHFFFAOYSA-N

Formula: C11H17NO2

SMILES: COc1ccc(OC)c(CC(C)N)c1

Mol. weight [g/mol]: 195.26

CAS: 2801-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-11.10	kJ/mol	Joback Method
hf	-292.71	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	604.65	K	Joback Method
tc	818.55	K	Joback Method
tf	377.91	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.34	J/mol×K	604.65	Joback Method
cpg	428.28	J/mol×K	640.30	Joback Method

cpg	442.45	J/mol×K	675.95	Joback Method
cpg	455.85	J/mol×K	711.60	Joback Method
cpg	468.48	J/mol×K	747.25	Joback Method
cpg	480.33	J/mol×K	782.90	Joback Method
cpg	491.41	J/mol×K	818.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2801685&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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