

2,4-DIMETHOXYAMPHETAMINE

Other names:	Benzeneethanamine,2,4-dimethoxy-«alpha»-methyl
Inchi:	InChI=1S/C11H17NO2/c1-8(12)6-9-4-5-10(13-2)7-11(9)14-3/h4-5,7-8H,6,12H2,1-3H3
InchiKey:	DQWOZMUBHQPFFF-UHFFFAOYSA-N
Formula:	C11H17NO2
SMILES:	COc1ccc(CC(C)N)c(OC)c1
Mol. weight [g/mol]:	195.26

Physical Properties

Property code	Value	Unit	Source
hfus	21.56	kJ/mol	Joback Method
ie	7.40	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
tb	557.20	K	Cheméo Relay (1.0)

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

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=C23690133&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
tb:	Normal Boiling Point Temperature

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