2,3-DIMETHOXYAMPHETAMINE

Other names: Benzeneethanamine,2,3-dimethoxy-«alpha»-methyl-
Inchi: InChI=1S/C11H17NO2/c1-8(12)7-9-5-4-6-10(13-2)11(9)14-3/h4-6,8H,7,12H2,1-3H3
InchiKey: DHLWJXGSZDJWKK-UHFFFAOYSA-N
Formula: C11H17NO2
SMILES: COc1cccc(CC(C)N)c1OC
Mol. weight [g/mol]: 195.26

Physical Properties

Property code	Value	Unit	Source
hfus	21.56	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
tb	545.32	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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15402810&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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