2,6-DIMETHOXYAMPHETAMINE

Other names: Benzeneethanamine, 2,6-dimethoxy, «alpha»-methyl-
Inchi: InChI=1S/C11H17NO2/c1-8(12)7-9-10(13-2)5-4-6-11(9)14-3/h4-6,8H,7,12H2,1-3H3
InchiKey: OHGNLLDQBKOWJW-UHFFFAOYSA-N
Formula: C11H17NO2
SMILES: COc1cccc(OC)c1CC(C)N
Mol. weight [g/mol]: 195.26

Physical Properties

Property code	Value	Unit	Source
hfus	21.56	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Cheméo Relay (1.0)
ie	8.18 ± 0.06	eV	NIST Webbook
log10ws	-1.62		Cheméo Relay (1.0)
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
tb	551.69	K	Cheméo Relay (1.0)
tf	356.28	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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23690144&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):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point