VERATRYLAMINE

Other names:	Veratrylamine
	Benzenemethanamine, 3,4-dimethoxy-
	Benzylamine, 3,4-(dimethoxy)-
Inchi:	InChI=1S/C9H13NO2/c1-11-8-4-3-7(6-10)5-9(8)12-2/h3-5H,6,10H2,1-2H3
InchiKey:	DIVNUTGTTIRPQA-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	COc1ccc(CN)cc1OC
Mol. weight [g/mol]:	167.21

Physical Properties

Property code	Value	Unit	Source
hfus	19.90	kJ/mol	Joback Method
hvap	75.06	kJ/mol	Cheméo Relay (1.0)
ie	7.72	eV	Cheméo Relay (1.0)
log10ws	-1.24		Cheméo Relay (1.0)
logp	1.163		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
tb	545.81	K	Cheméo Relay (1.0)
tf	313.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.11	J/mol×K	559.33	Joback Method
cpg	330.99	J/mol×K	595.46	Joback Method
cpg	343.27	J/mol×K	631.58	Joback Method
cpg	354.93	J/mol×K	667.71	Joback Method
cpg	365.96	J/mol×K	703.83	Joback Method
cpg	376.37	J/mol×K	739.96	Joback Method
cpg	386.14	J/mol×K	776.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.20	K	1.60	NIST Webbook
tbrp	393.20	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5763611&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
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point