Benzenemethanamine, 2,3-dimethoxy-

Other names: 2,3-Dimethoxybenzylamine
Inchi: InChI=1S/C9H13NO2/c1-11-8-5-3-4-7(6-10)9(8)12-2/h3-5H,6,10H2,1-2H3
InchiKey: LVMPWFJVYMXSNY-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: COc1cccc(CN)c1OC
Mol. weight [g/mol]: 167.21
CAS: 4393-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-25.50	kJ/mol	Joback Method
hf	-246.15	kJ/mol	Joback Method
hfus	19.90	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.163		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	559.33	K	Joback Method
tc	776.09	K	Joback Method
tf	370.37	K	Joback Method
vc	0.496	m3/kmol	Joback Method

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	410.20	K	1.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4393093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume