Methoxamine

Other names:	Benzenemethanol, «alpha»-(1-aminoethyl)-2,5-dimethoxy-
	Benzyl alcohol, «alpha»-(1-aminoethyl)-2,5-dimethoxy-
	Methoxamin
	Pseudomethoxamine
	(.+/-.)-«alpha»-(1-Aminoethyl)-2,5-dimethoxybenzyl alcohol
	2,5-Dimethoxynorephedrine
	Benzyl alcohol, alpha-(1-aminoethyl)-2,5-dimethoxy-
Inchi:	InChI=1S/C11H17NO3/c1-7(12)11(13)9-6-8(14-2)4-5-10(9)15-3/h4-7,11,13H,12H2,1-3H3
InchiKey:	WJAJPNHVVFWKKL-UHFFFAOYSA-N
Formula:	C11H17NO3
SMILES:	COc1ccc(OC)c(C(O)C(C)N)c1
Mol. weight [g/mol]:	211.26
CAS:	390-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-150.36	kJ/mol	Joback Method
hf	-450.22	kJ/mol	Joback Method
hfus	22.12	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.084		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	696.39	K	Joback Method
tc	900.21	K	Joback Method
tf	423.73	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.47	J/mol×K	696.39	Joback Method
cpg	481.04	J/mol×K	730.36	Joback Method
cpg	492.88	J/mol×K	764.33	Joback Method
cpg	503.99	J/mol×K	798.30	Joback Method
cpg	514.37	J/mol×K	832.27	Joback Method
cpg	524.01	J/mol×K	866.24	Joback Method
cpg	532.93	J/mol×K	900.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C390283&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume