

1-Propanamine, 3-methoxy-

Other names:	.gamma.-methoxypropylamine 1-Methoxy-3-aminopropane 1-amino-3-methoxypropane 3-Aminopropyl methyl ether 3-MPA 3-Methoxy-1-propanamine 3-Methoxy-1-propylamine 3-Methoxy-n-propylamine 3-Methoxypropylamine 3-methoxypropylamine NSC 552 Propanolamine methyl ether propylamine, 3-methoxy- «gamma»-Methoxypropylamine
Inchi:	InChI=1S/C4H11NO/c1-6-4-2-3-5/h2-5H2,1H3
InchiKey:	FAXDZWQIWUSWJH-UHFFFAOYSA-N
Formula:	C4H11NO
SMILES:	COCCCN
Mol. weight [g/mol]:	89.14
CAS:	5332-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-55.75	kJ/mol	Joback Method
hf	-224.32	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hvap	37.55	kJ/mol	Joback Method
ie	9.37 ± 0.12	eV	NIST Webbook
log10ws	-0.02		Crippen Method
logp	-0.018		Crippen Method
mcvol	83.070	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
sl	257.60	J/molxK	NIST Webbook
tb	385.87	K	Joback Method
tc	567.91	K	Joback Method
tf	197.45 ± 0.15	K	NIST Webbook
tf	197.20 ± 0.20	K	NIST Webbook

tf	135.00	K	NIST Webbook
vc	0.306	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.63	J/mol×K	385.87	Joback Method
cpg	168.06	J/mol×K	416.21	Joback Method
cpg	176.23	J/mol×K	446.55	Joback Method
cpg	184.16	J/mol×K	476.89	Joback Method
cpg	191.83	J/mol×K	507.23	Joback Method
cpg	199.25	J/mol×K	537.57	Joback Method
cpg	206.42	J/mol×K	567.91	Joback Method
cpl	225.52	J/mol×K	298.15	NIST Webbook
hvapt	44.50	kJ/mol	334.00	NIST Webbook
pvap	1.39	kPa	292.94	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.70	kPa	282.42	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.55	kPa	278.95	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	1.61	kPa	295.29	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.23	kPa	300.81	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.91	kPa	298.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.77	kPa	304.54	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	3.31	kPa	307.79	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	4.66	kPa	314.16	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	5.56	kPa	317.57	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.01	kPa	287.91	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.82	kPa	297.33	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.91	kPa	298.13	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	97.70	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576
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=C5332730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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