Carbamic acid, methyl ester

Other names:	Methyl carbamate
	Methylester kyseliny karbaminove
	Methylkarbamat
	Methylurethan
	Methylurethane
	NCI-C55594
	Urethylane
	o-methyl carbamate
Inchi:	InChI=1S/C2H5NO2/c1-5-2(3)4/h1H3,(H2,3,4)
InchiKey:	GTCAXTIRRLKXRU-UHFFFAOYSA-N
Formula:	C2H5NO2
SMILES:	COC(N)=O
Mol. weight [g/mol]:	75.07
CAS:	598-55-0

Physical Properties

Property code	Value	Unit	Source
gf	-201.51	kJ/mol	Joback Method
hf	-425.30	kJ/mol	NIST Webbook
hfl	-472.70	kJ/mol	NIST Webbook
hfus	8.92	kJ/mol	Joback Method
hvap	47.30 ± 1.70	kJ/mol	NIST Webbook
log10ws	0.97		Aqueous Solubility Prediction Method
logp	-0.288		Crippen Method
mcvol	56.460	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
tb	450.20	K	NIST Webbook
tc	592.23	K	Joback Method
tf	328.60 ± 0.50	K	NIST Webbook
tf	327.65	K	Aqueous Solubility Prediction Method
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.95	J/mol×K	592.23	Joback Method
cpg	107.78	J/mol×K	427.02	Joback Method
cpg	112.47	J/mol×K	460.06	Joback Method
cpg	117.04	J/mol×K	493.10	Joback Method
cpg	121.48	J/mol×K	526.14	Joback Method
cpg	125.79	J/mol×K	559.19	Joback Method
cpg	102.98	J/mol×K	393.98	Joback Method
hfust	16.70	kJ/mol	328.60	NIST Webbook
hfust	16.70	kJ/mol	328.60	NIST Webbook
hfust	16.70	kJ/mol	328.60	NIST Webbook
hsubt	74.50 ± 0.80	kJ/mol	296.00	NIST Webbook
hvapt	73.60	kJ/mol	298.15	The enthalpies of formation of alkyl carbamates: Experimental and computational redetermination
hvapt	45.70	kJ/mol	360.50	NIST Webbook
pvap	1.31	kPa	341.45	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	13.99	kPa	393.75	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures

pvap	12.39	kPa	390.50	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	10.96	kPa	387.17	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	9.83	kPa	384.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	7.14	kPa	377.23	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	6.23	kPa	373.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	

pvap	5.42	kPa	371.70	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	4.48	kPa	367.00	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	4.19	kPa	364.43	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	3.55	kPa	360.75	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	2.50	kPa	356.06	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures

pvap	1.91	kPa	350.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
sfust	51.00	J/mol×K	328.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	1.90	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The enthalpies of formation of alkyl carbamates: Experimental and computational redetermination:	https://www.doi.org/10.1016/j.jct.2012.08.018
Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures:	https://www.doi.org/10.1021/je400551d
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume