Carbamic acid, phenyl-, methyl ester

Other names:	Carbanilic acid, methyl ester
	Methyl N-phenylurethane
	Methyl carbanilate
	Methyl phenylurethane
	N-Phenylcarbamic acid methyl ester
	methyl N-phenylcarbamate
	methyl phenylcarbamate
Inchi:	InChI=1S/C8H9NO2/c1-11-8(10)9-7-5-3-2-4-6-7/h2-6H,1H3,(H,9,10)
InchiKey:	IAGUPODHENSJEZ-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	COC(=O)Nc1ccccc1
Mol. weight [g/mol]:	151.16
CAS:	2603-10-3

Physical Properties

Property code	Value	Unit	Source
chs	-4248.00 ± 2.00	kJ/mol	NIST Webbook
gf	-15.64	kJ/mol	Joback Method
hf	-163.25	kJ/mol	Joback Method
hfus	18.40	kJ/mol	Joback Method
hvap	51.27	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.865		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1315.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	535.58	K	Joback Method
tc	755.73	K	Joback Method
tf	325.00 ± 1.00	K	NIST Webbook

vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.41	J/mol×K	755.73	Joback Method
cpg	309.03	J/mol×K	719.03	Joback Method
cpg	300.01	J/mol×K	682.34	Joback Method
cpg	290.31	J/mol×K	645.65	Joback Method
cpg	279.94	J/mol×K	608.96	Joback Method
cpg	268.87	J/mol×K	572.27	Joback Method
cpg	257.09	J/mol×K	535.58	Joback Method
cps	203.30	J/mol×K	298.00	NIST Webbook
hfust	14.55	kJ/mol	325.00	NIST Webbook
hfust	14.56	kJ/mol	325.00	NIST Webbook
hfust	14.56	kJ/mol	325.00	NIST Webbook
pvap	0.33	kPa	380.65	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.56	kPa	390.35	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.59	kPa	391.76	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures

pvap	0.65	kPa	394.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.72	kPa	395.80	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.31	kPa	379.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.79	kPa	397.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.94	kPa	399.63	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures

pvap	0.94	kPa	399.83	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	1.06	kPa	402.15	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	1.29	kPa	409.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	1.54	kPa	412.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
pvap	1.97	kPa	415.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	

pvap	2.13	kPa	418.45	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.50	kPa	387.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.25	kPa	376.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.22	kPa	374.46	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.21	kPa	372.50	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures

pvap	0.45	kPa	385.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.39	kPa	383.31	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
pvap	0.79	kPa	397.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures
sfust	44.80	J/mol×K	325.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2603103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume