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
рс	3925.85	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	535.58	К	Joback Method
tc	755.73	К	Joback Method
tf	325.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source	
cpg	257.09	J/mol×K	535.58	Joback Method	
cpg	268.87	J/mol×K	572.27	Joback Method	
cpg	279.94	J/mol×K	608.96	Joback Method	
cpg	290.31	J/mol×K	645.65	Joback Method	
cpg	300.01	J/mol×K	682.34	Joback Method	
cpg	309.03	J/mol×K	719.03	Joback Method	
cpg	317.41	J/mol×K	755.73	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	
рvар	0.39	kPa	383.31	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate	
				F Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	0.22	kPa	374.46	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	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	0.31	kPa	379.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	0.33	kPa	380.65	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	0.21	kPa	372.50	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	0.45	kPa	385.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	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	0.56	kPa	390.35	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different	
	0.50		004 70	Pressures	
pvap	0.59	кРа	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	
рvар	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	0.79	kPa	397.05	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	0.94	kPa	399.63	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different	
рvар	0.94	kPa	399.83	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	1.06	kPa	402.15	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	1.29	kPa	409.85	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	

рvар	1.54	kPa	412.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	1.97	kPa	415.90	Determination and Modeling of Isobaric Vapor Liquid Equilibria for the Methylcarbamate + Methyl-N-phenyl Carbamate System at Different Pressures	
рvар	2.13	kPa	418.45	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:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Modeling of Isobaric	https://www.doi.org/10.1021/je400551d
wapor Liguid Equilibria for the	https://en.wikipedia.org/wiki/Joback_method
Carbamate System at Different	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2603103&Units=SI

Legend

Standard solid enthalpy of combustion

chs:

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

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