

Carbamic acid, methyl-, ethyl ester

Other names:	Ethyl methylcarbamate Ethyl N-methylcarbamate Methylurethane N-Methylurethan N-Methylurethane Methylcarbamic acid, ethyl ester Ethylester kyseliny methylkarbaminove CH3NHCOOC2H5
Inchi:	InChI=1S/C4H9NO2/c1-3-7-4(6)5-2/h3H2,1-2H3,(H,5,6)
InchiKey:	SURZCVYFPAXNGN-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CCOC(=O)NC
Mol. weight [g/mol]:	103.12
CAS:	105-40-8

Physical Properties

Property code	Value	Unit	Source
affp	888.80	kJ/mol	NIST Webbook
basg	857.80	kJ/mol	NIST Webbook
gf	-161.73	kJ/mol	Joback Method
hf	-317.22	kJ/mol	Joback Method
hfus	14.00	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.362		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	867.00		NIST Webbook
ripol	1433.00		NIST Webbook
tb	443.20	K	NIST Webbook
tc	601.82	K	Joback Method
tf	259.66	K	Joback Method
vc	0.319	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.98	J/mol×K	417.38	Joback Method
cpg	172.03	J/mol×K	448.12	Joback Method
cpg	179.82	J/mol×K	478.86	Joback Method
cpg	187.35	J/mol×K	509.60	Joback Method
cpg	194.62	J/mol×K	540.34	Joback Method
cpg	201.63	J/mol×K	571.08	Joback Method
cpg	208.36	J/mol×K	601.82	Joback Method
hvapt	51.70	kJ/mol	371.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105408&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

affp:	Proton affinity
basg:	Gas basicity
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

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_{brp}:	Boiling point at reduced pressure
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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