ETHYL N-METHYLCARBAMATE

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

Physical Properties

Property code	Value	Unit	Source
af	0.4658		Cheméo Relay (1.0)
affp	888.80	kJ/mol	NIST Webbook
basg	857.80	kJ/mol	NIST Webbook
gf	-161.73	kJ/mol	Joback Method
hf	-452.60	kJ/mol	Cheméo Relay (1.0)
hfus	14.00	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	0.06		Cheméo Relay (1.0)
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	599.90	K	Cheméo Relay (1.0)
tf	264.84	K	Cheméo Relay (1.0)
vc	0.318	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105408&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume