

Carbamic acid, ethyl-, ethyl ester

Other names:	Ethyl ethylcarbamate N-Ethylurethane Ethyl N-ethylcarbamate Ethylcarbamic acid, ethyl ester
Inchi:	InChI=1S/C5H11NO2/c1-3-6-5(7)8-4-2/h3-4H2,1-2H3,(H,6,7)
InchiKey:	GZXSDYYWLZERLF-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CCNC(=O)OCC
Mol. weight [g/mol]:	117.15
CAS:	623-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-153.31	kJ/mol	Joback Method
hf	-337.86	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	42.32	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	0.752		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	458.40 ± 0.30	K	NIST Webbook
tc	623.20	K	Joback Method
tf	270.93	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.38	J/mol×K	440.26	Joback Method
cpg	210.79	J/mol×K	470.75	Joback Method
cpg	219.87	J/mol×K	501.24	Joback Method
cpg	228.63	J/mol×K	531.73	Joback Method
cpg	237.06	J/mol×K	562.22	Joback Method

cpg	245.16	J/mol×K	592.71	Joback Method
cpg	252.94	J/mol×K	623.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	2.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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