Urethane

Other names:	A 11032 Aethylcarbamat Aethylurethan Carbamic acid, ethyl ester Carbamidsaeure-aethylester ETHYL CARBAMATE Estane 5703 Ethyl ester of carbamic acid Ethyl urethan Ethyl urethane Ethylester kyseliny karbaminove LEUCETHANE Leucothane NH2COOC2H5 NSC 746 O-ETHYLURETHANE Pracarbamin Pracarbamine Rcra waste number U238 U-Compound Uretan Uretan etylowy Urethan X 41 ethyl aminoformate ethylurethane o-ethyl carbamate
Inchi:	InChI=1S/C3H7NO2/c1-2-6-3(4)5/h2H2,1H3,(H2,4,5)
InchiKey:	JOYRKODLDBILNP-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	CCOC(N)=O
Mol. weight [g/mol]:	89.09
CAS:	51-79-6

Physical Properties

Property code	Value	Unit	Source

chs	-1663.80	kJ/mol	NIST Webbook
gf	-193.09	kJ/mol	Joback Method
hf	-446.30	kJ/mol	NIST Webbook
hfl	-497.30	kJ/mol	NIST Webbook
hfs	-517.10	kJ/mol	NIST Webbook
hfus	11.51	kJ/mol	Joback Method
hsub	76.30	kJ/mol	NIST Webbook
hvap	51.00 ± 2.50	kJ/mol	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
log10ws	0.85		Aqueous Solubility Prediction Method
log10ws	0.85		Estimated Solubility Method
logp	0.102		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	838.00		NIST Webbook
tb	456.20	K	NIST Webbook
tb	458.40 ± 0.60	K	NIST Webbook
tb	458.40	K	KDB
tc	613.38	K	Joback Method
tf	321.34	K	KDB
tf	321.90	K	Aqueous Solubility Prediction Method
tt	321.41 ± 0.02	K	NIST Webbook
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.18	J/mol×K	613.38	Joback Method
cpg	142.88	J/mol×K	449.61	Joback Method
cpg	149.16	J/mol×K	482.37	Joback Method
cpg	155.23	J/mol×K	515.12	Joback Method
cpg	161.10	J/mol×K	547.87	Joback Method
cpg	166.75	J/mol×K	580.63	Joback Method
cpg	136.41	J/mol×K	416.86	Joback Method
cps	156.43	J/mol×K	300.00	NIST Webbook
hfust	16.79	kJ/mol	321.41	NIST Webbook
hfust	20.90	kJ/mol	321.70	NIST Webbook
hfust	15.23	kJ/mol	321.90	NIST Webbook

hsubt	77.70	kJ/mol	264.50	NIST Webbook
hsubt	89.10 ± 0.80	kJ/mol	299.50	NIST Webbook
hsubt	71.90	kJ/mol	322.00	NIST Webbook
hvapt	77.70	kJ/mol	298.15	The enthalpies of formation of alkyl carbamates: Experimental and computational redetermination
hvapt	56.60	kJ/mol	397.50	NIST Webbook
pvap	0.88	kPa	322.60	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	1.29	kPa	337.20	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	1.49	kPa	342.30	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	1.96	kPa	352.50	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	2.38	kPa	362.60	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K

pvap	2.95	kPa	371.70	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
sfust	52.25	J/mol×K	321.41	NIST Webbook
sfust	64.80	J/mol×K	321.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.20583e+01
Coeff. B	-1.00894e+04
Coeff. C	-1.08907e+01
Coeff. D	6.38522e-06
Temperature range (K), min.	338.15
Temperature range (K), max.	457.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1464.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51796&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1464
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K:	https://www.doi.org/10.1021/je030222n
The enthalpies of formation of alkyl carbamates: Experimental and computational redetermination:	https://www.doi.org/10.1016/j.jct.2012.08.018

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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume