Acetic acid, diethyl-

Other names:	(C2H5)2CHCOOH
	2-ETHYL BUTYRIC ACID
	2-Ethyl-n-butyric acid
	2-Ethylbutanoic acid
	2-Ethylbutyric acid
	3-Pentanecarboxylic acid
	Butanoic acid, 2-ethyl-
	Butyric acid, 2-ethyl-
	Diethylacetic acid
	Kyselina diethyloctova
	NSC 11765
	«alpha»-Ethylbutyric acid
	Â«alphaÂ»-Ethylbutyric acid
Inchi:	InChI=1S/C6H12O2/c1-3-5(4-2)6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
InchiKey:	OXQGTIUCKGYOAA-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC(CC)C(=O)O
Mol. weight [g/mol]:	116.16
CAS:	88-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-268.54	kJ/mol	Joback Method
hf	-437.26	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-0.81		Aqueous Solubility Prediction Method
logp	1.507		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	467.65 ± 3.00	K	NIST Webbook
tb	463.65 ± 2.00	K	NIST Webbook
tb	462.65 ± 4.00	K	NIST Webbook
tb	467.15 ± 0.70	K	NIST Webbook
tb	466.15 ± 3.00	K	NIST Webbook
tb	467.20	K	NIST Webbook

tb	467.35	K	NIST Webbook
tb	409.90 ± 2.50	K	NIST Webbook
tb	469.15 ± 3.00	K	NIST Webbook
tc	657.19	K	Joback Method
tf	241.35 ± 0.50	K	NIST Webbook
tf	258.20 ± 0.60	K	NIST Webbook
tf	249.75	K	Aqueous Solubility Prediction Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.38	J/mol×K	657.19	Joback Method
cpg	266.02	J/mol×K	628.04	Joback Method
cpg	258.31	J/mol×K	598.89	Joback Method
cpg	250.24	J/mol×K	569.74	Joback Method
cpg	241.81	J/mol×K	540.59	Joback Method
cpg	233.01	J/mol×K	511.44	Joback Method
cpg	223.83	J/mol×K	482.29	Joback Method
dvisc	0.0437428	Pa×s	253.13	Joback Method
dvisc	0.0001967	Pa×s	482.29	Joback Method
dvisc	0.0003288	Pa×s	444.10	Joback Method
dvisc	0.0006050	Pa×s	405.90	Joback Method
dvisc	0.0012640	Pa×s	367.71	Joback Method
dvisc	0.0031323	Pa×s	329.52	Joback Method
dvisc	0.0098475	Pa×s	291.32	Joback Method
hvapt	58.20	kJ/mol	419.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	2.40	NIST Webbook
tbrp	363.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62109e+01
Coeff. B	-4.48107e+03
Coeff. C	-7.34520e+01
Temperature range (K), min.	354.87
Temperature range (K), max.	484.58

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.58114e+01
Coeff. B	-9.71131e+03
Coeff. C	-8.26984e+00
Coeff. D	1.76223e-06
Temperature range (K), min.	258.15
Temperature range (K), max.	655.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88095&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=940

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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