

Acetic acid, ethoxy-

Other names:	Ethoxyacetic acid 2-Ethoxyacetic acid
Inchi:	InChI=1S/C4H8O3/c1-2-7-3-4(5)6/h2-3H2,1H3,(H,5,6)
InchiKey:	YZGQDNOIGFBYKF-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	CCOCC(=O)O
Mol. weight [g/mol]:	104.10
CAS:	627-03-2

Physical Properties

Property code	Value	Unit	Source
chl	-2069.00 ± 0.50	kJ/mol	NIST Webbook
gf	-387.94	kJ/mol	Joback Method
hf	-522.92	kJ/mol	Joback Method
hfl	-648.40 ± 0.50	kJ/mol	NIST Webbook
hfus	12.99	kJ/mol	Joback Method
hvap	50.33	kJ/mol	Joback Method
log10ws	0.32		Crippen Method
logp	0.107		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	479.70	K	NIST Webbook
tc	632.96	K	Joback Method
tf	267.82	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.81	J/molxK	632.96	Joback Method
cpg	165.79	J/molxK	459.39	Joback Method
cpg	172.31	J/molxK	488.32	Joback Method
cpg	178.62	J/molxK	517.25	Joback Method
cpg	184.73	J/molxK	546.17	Joback Method

cpg	190.63	J/mol×K	575.10	Joback Method
cpg	196.32	J/mol×K	604.03	Joback Method
dvisc	0.0002191	Paxs	459.39	Joback Method
dvisc	0.0164842	Paxs	267.82	Joback Method
dvisc	0.0054671	Paxs	299.75	Joback Method
dvisc	0.0022425	Paxs	331.68	Joback Method
dvisc	0.0010757	Paxs	363.61	Joback Method
dvisc	0.0005809	Paxs	395.53	Joback Method
dvisc	0.0003440	Paxs	427.46	Joback Method
hvapt	69.10	kJ/mol	295.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.70	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627032&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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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