Acetic acid, 2-ethylbutyl ester

Other names: 2-Ethylbutyl acetate
Inchi: InChI=1S/C8H16O2/c1-4-8(5-2)6-10-7(3)9/h8H,4-6H2,1-3H3
InchiKey: HQLKZWRSOHTERR-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(CC)COC(C)=O
Mol. weight [g/mol]: 144.21
CAS: 10031-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	957.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1205.00		NIST Webbook
tb	432.00	K	NIST Webbook
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56281e+01
Coeff. B	-4.07075e+03
Coeff. C	-6.22610e+01
Temperature range (K), min.	327.62
Temperature range (K), max.	456.84

Sources

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=C10031875&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
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