Ethanol, 2-allyloxy, acetate

Inchi: InChI=1S/C7H12O3/c1-3-4-9-5-6-10-7(2)8/h3H,1,4-6H2,2H3
InchiKey: UPPPRUXHPDMSCT-UHFFFAOYSA-N
Formula: C7H12O3
SMILES: C=CCOCCOC(C)=O
Mol. weight [g/mol]: 144.17

Physical Properties

Property code	Value	Unit	Source
gf	-243.02	kJ/mol	Joback Method
hf	-439.40	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.752		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	980.00		NIST Webbook
tb	454.95	K	Joback Method
tc	634.51	K	Joback Method
tf	261.28	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.27	J/mol×K	454.95	Joback Method
cpg	255.58	J/mol×K	484.88	Joback Method
cpg	265.55	J/mol×K	514.80	Joback Method
cpg	275.20	J/mol×K	544.73	Joback Method
cpg	284.52	J/mol×K	574.65	Joback Method
cpg	293.49	J/mol×K	604.58	Joback Method
cpg	302.12	J/mol×K	634.51	Joback Method
dvisc	0.0022166	Pa×s	261.28	Joback Method
dvisc	0.0012324	Pa×s	293.56	Joback Method
dvisc	0.0007698	Pa×s	325.84	Joback Method
dvisc	0.0005234	Pa×s	358.12	Joback Method
dvisc	0.0003793	Pa×s	390.39	Joback Method
dvisc	0.0002887	Pa×s	422.67	Joback Method
dvisc	0.0002284	Pa×s	454.95	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R151981&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume