Allyl levulinate

Other names: Levulinic acid, 2-propenyl ester
Inchi: InChI=1S/C8H12O3/c1-3-6-11-8(10)5-4-7(2)9/h3H,1,4-6H2,2H3
InchiKey: NETFSRNRGBJVMU-UHFFFAOYSA-N
Formula: C8H12O3
SMILES: C=CCOC(=O)CCC(C)=O
Mol. weight [g/mol]: 156.18
CAS: 1070-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-258.52	kJ/mol	Joback Method
hf	-440.40	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	48.63	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.085		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1743.00		NIST Webbook
tb	509.28	K	Joback Method
tc	697.68	K	Joback Method
tf	300.25	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.56	J/mol×K	509.28	Joback Method
cpg	291.49	J/mol×K	540.68	Joback Method
cpg	301.95	J/mol×K	572.08	Joback Method

cpg	311.94	J/mol×K	603.48	Joback Method
cpg	321.46	J/mol×K	634.88	Joback Method
cpg	330.53	J/mol×K	666.28	Joback Method
cpg	339.15	J/mol×K	697.68	Joback Method
dvisc	0.0025755	Pa×s	300.25	Joback Method
dvisc	0.0014733	Pa×s	335.09	Joback Method
dvisc	0.0009363	Pa×s	369.93	Joback Method
dvisc	0.0006433	Pa×s	404.76	Joback Method
dvisc	0.0004691	Pa×s	439.60	Joback Method
dvisc	0.0003583	Pa×s	474.44	Joback Method
dvisc	0.0002840	Pa×s	509.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070355&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume