

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	1114.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1114.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1694.00		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/molxK	509.28	Joback Method
cpg	330.53	J/molxK	666.28	Joback Method
cpg	321.46	J/molxK	634.88	Joback Method

cpg	311.94	J/molxK	603.48	Joback Method
cpg	301.95	J/molxK	572.08	Joback Method
cpg	291.49	J/molxK	540.68	Joback Method
cpg	339.15	J/molxK	697.68	Joback Method
dvisc	0.0002840	Paxs	509.28	Joback Method
dvisc	0.0003583	Paxs	474.44	Joback Method
dvisc	0.0004691	Paxs	439.60	Joback Method
dvisc	0.0006433	Paxs	404.76	Joback Method
dvisc	0.0009363	Paxs	369.93	Joback Method
dvisc	0.0014733	Paxs	335.09	Joback Method
dvisc	0.0025755	Paxs	300.25	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/ci9903071
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

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