

Levulinic acid, ethyl ester, diethyl acetal

Inchi:	InChI=1S/C11H22O4/c1-5-13-10(12)8-9-11(4,14-6-2)15-7-3/h5-9H2,1-4H3
InchiKey:	JWMRPSYVFUZQCJ-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CCOC(=O)CCC(C)(OCC)OCC
Mol. weight [g/mol]:	218.29
CAS:	92557-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-399.34	kJ/mol	Joback Method
hf	-788.36	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	52.76	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.119		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	568.98	K	Joback Method
tc	747.80	K	Joback Method
tf	332.77	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.40	J/molxK	568.98	Joback Method
cpg	542.70	J/molxK	717.99	Joback Method
cpg	529.92	J/molxK	688.19	Joback Method
cpg	516.50	J/molxK	658.39	Joback Method
cpg	502.44	J/molxK	628.59	Joback Method
cpg	487.74	J/molxK	598.78	Joback Method
cpg	554.85	J/molxK	747.80	Joback Method
dvisc	0.0001206	Paxs	568.98	Joback Method
dvisc	0.0001607	Paxs	529.61	Joback Method

dvisc	0.0002244	Paxs	490.24	Joback Method
dvisc	0.0003319	Paxs	450.88	Joback Method
dvisc	0.0005293	Paxs	411.51	Joback Method
dvisc	0.0009317	Paxs	372.14	Joback Method
dvisc	0.0018745	Paxs	332.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92557396&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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