Pentanoic acid, 4-oxo-, propyl ester

Other names: n-Propyl levulinate
Propyl 4-oxopentanoate
Propyl levulinate
Inchi: InChI=1S/C8H14O3/c1-3-6-11-8(10)5-4-7(2)9/h3-6H2,1-2H3
InchiKey: QOSMNYMQXIVWKY-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCCOC(=O)CCC(C)=O
Mol. weight [g/mol]: 158.19
CAS: 645-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-346.36	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.309		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1064.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1663.00		NIST Webbook
tb	512.60	K	Joback Method
tc	697.35	K	Joback Method
tf	302.01	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.67	J/mol×K	512.60	Joback Method

cpg	310.25	J/mol×K	543.39	Joback Method
cpg	321.37	J/mol×K	574.18	Joback Method
cpg	332.03	J/mol×K	604.98	Joback Method
cpg	342.23	J/mol×K	635.77	Joback Method
cpg	351.97	J/mol×K	666.56	Joback Method
cpg	361.25	J/mol×K	697.35	Joback Method
dvisc	0.0015339	Pa×s	337.11	Joback Method
dvisc	0.0027356	Pa×s	302.01	Joback Method
dvisc	0.0009592	Pa×s	372.21	Joback Method
dvisc	0.0006504	Pa×s	407.31	Joback Method
dvisc	0.0004690	Pa×s	442.40	Joback Method
dvisc	0.0003549	Pa×s	477.50	Joback Method
dvisc	0.0002790	Pa×s	512.60	Joback Method
hvapt	56.30	kJ/mol	413.50	NIST Webbook
hvapt	54.00	kJ/mol	436.00	NIST Webbook

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=C645670&Units=SI
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
hvapt: Enthalpy of vaporization at a given temperature
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