Pentanoic acid, 4-oxo-, pentyl ester

Other names:	n-Amyl levulinate
	Pentyl 4-oxopentanoate
	Pentyl levulinate
	Levulinic acid, pentyl ester
	pentyl 4-oxovalerate
Inchi:	InChI=1S/C10H18O3/c1-3-4-5-8-13-10(12)7-6-9(2)11/h3-8H2,1-2H3
InchiKey:	NLDFWNCRMVSDMC-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCCCCOC(=O)CCC(C)=O
Mol. weight [g/mol]:	186.25
CAS:	20279-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-329.52	kJ/mol	Joback Method
hf	-607.11	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.089		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1324.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	558.36	K	Joback Method
tc	739.30	K	Joback Method
tf	324.55	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.38	J/mol×K	709.15	Joback Method
cpg	461.96	J/mol×K	739.30	Joback Method
cpg	390.21	J/mol×K	558.36	Joback Method
cpg	403.56	J/mol×K	588.52	Joback Method
cpg	416.35	J/mol×K	618.67	Joback Method
cpg	428.57	J/mol×K	648.83	Joback Method
cpg	440.25	J/mol×K	678.99	Joback Method
dvisc	0.0002364	Pa×s	558.36	Joback Method
dvisc	0.0003038	Pa×s	519.39	Joback Method
dvisc	0.0026272	Pa×s	324.55	Joback Method
dvisc	0.0014182	Pa×s	363.52	Joback Method
dvisc	0.0008627	Pa×s	402.49	Joback Method
dvisc	0.0005729	Pa×s	441.46	Joback Method
dvisc	0.0004066	Pa×s	480.42	Joback Method
hvapt	56.20	kJ/mol	466.00	NIST Webbook
hvapt	66.30	kJ/mol	440.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20279496&Units=SI

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