

Pentanoic acid, 3-methyl-4-oxo-

Other names:	3-Methyl-4-oxopentanoic acid Levulinic acid, 3-methyl 3-Methyllevulinic acid
Inchi:	InChI=1S/C6H10O3/c1-4(5(2)7)3-6(8)9/h4H,3H2,1-2H3,(H,8,9)
InchiKey:	NFIWUVRBASXMGK-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC(=O)C(C)CC(=O)O
Mol. weight [g/mol]:	130.14
CAS:	6628-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-397.46	kJ/mol	Joback Method
hf	-549.84	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	58.73	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.686		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	536.16	K	Joback Method
tc	720.16	K	Joback Method
tf	303.06	K	Joback Method
vc	0.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.83	J/mol×K	536.16	Joback Method
cpg	245.27	J/mol×K	566.83	Joback Method
cpg	253.30	J/mol×K	597.49	Joback Method
cpg	260.95	J/mol×K	628.16	Joback Method
cpg	268.22	J/mol×K	658.83	Joback Method
cpg	275.12	J/mol×K	689.50	Joback Method

cpg	281.66	J/mol×K	720.16	Joback Method
dvisc	0.0145779	Paxs	303.06	Joback Method
dvisc	0.0045167	Paxs	341.91	Joback Method
dvisc	0.0017774	Paxs	380.76	Joback Method
dvisc	0.0008313	Paxs	419.61	Joback Method
dvisc	0.0004422	Paxs	458.46	Joback Method
dvisc	0.0002596	Paxs	497.31	Joback Method
dvisc	0.0001647	Paxs	536.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6628791&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
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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