3-Pentenoic acid

Inchi: InChI=1S/C5H8O2/c1-2-3-4-5(6)7/h2-3H,4H2,1H3,(H,6,7)
InchiKey: UIUWNILCHFBLEQ-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: CC=CCC(=O)O
Mol. weight [g/mol]: 100.12
CAS: 5204-64-8

Physical Properties

Property code	Value	Unit	Source
chl	-2676.10 ± 2.10	kJ/mol	NIST Webbook
gf	-194.30	kJ/mol	Joback Method
hf	-294.12	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	50.11	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	464.01	K	Joback Method
tc	644.72	K	Joback Method
tf	251.78	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.69	J/mol×K	464.01	Joback Method
cpg	173.98	J/mol×K	494.13	Joback Method
cpg	180.90	J/mol×K	524.25	Joback Method
cpg	187.47	J/mol×K	554.36	Joback Method
cpg	193.71	J/mol×K	584.48	Joback Method
cpg	199.64	J/mol×K	614.60	Joback Method
cpg	205.26	J/mol×K	644.72	Joback Method
dvisc	0.0276361	Pa×s	251.78	Joback Method

dvisc	0.0072921	Pa×s	287.15	Joback Method
dvisc	0.0025772	Pa×s	322.52	Joback Method
dvisc	0.0011187	Pa×s	357.89	Joback Method
dvisc	0.0005643	Pa×s	393.27	Joback Method
dvisc	0.0003187	Pa×s	428.64	Joback Method
dvisc	0.0001963	Pa×s	464.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.00 ± 1.00	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55457e+01
Coeff. B	-4.33606e+03
Coeff. C	-7.07400e+01
Temperature range (K), min.	354.92
Temperature range (K), max.	494.42

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5204648&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

chl:	Standard liquid enthalpy of combustion
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume