4-Pentenoic acid

Other names:	4 PA
	Allylacetic acid
	Pent-4-enoic acid
	«delta»4-Pentenoic acid
	Â«deltaÂ»4-Pentenoic acid
Inchi:	InChI=1S/C5H8O2/c1-2-3-4-5(6)7/h2H,1,3-4H2,(H,6,7)
InchiKey:	HVAMZGADVCBITI-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	C=CCCC(=O)O
Mol. weight [g/mol]:	100.12
CAS:	591-80-0

Physical Properties

Property code	Value	Unit	Source
chl	-2680.30 ± 2.50	kJ/mol	NIST Webbook
gf	-186.68	kJ/mol	Joback Method
hf	-285.91	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	65.80 ± 0.40	kJ/mol	NIST Webbook
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4074.47 ± 100.00	kPa	NIST Webbook
tb	461.70	K	NIST Webbook
tc	659.75 ± 3.00	K	NIST Webbook
tf	255.10	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.58	J/mol×K	456.53	Joback Method
cpg	174.70	J/mol×K	485.87	Joback Method
cpg	181.49	J/mol×K	515.21	Joback Method

cpg	187.98	J/mol×K	544.55	Joback Method
cpg	194.17	J/mol×K	573.90	Joback Method
cpg	200.07	J/mol×K	603.24	Joback Method
cpg	205.68	J/mol×K	632.58	Joback Method
dvisc	0.0255100	Pa×s	255.10	Joback Method
dvisc	0.0075116	Pa×s	288.67	Joback Method
dvisc	0.0028535	Pa×s	322.24	Joback Method
dvisc	0.0013013	Pa×s	355.81	Joback Method
dvisc	0.0006794	Pa×s	389.39	Joback Method
dvisc	0.0003933	Pa×s	422.96	Joback Method
dvisc	0.0002467	Pa×s	456.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36445e+01
Coeff. B	-3.16277e+03
Coeff. C	-1.17145e+02
Temperature range (K), min.	353.93
Temperature range (K), max.	496.69

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591800&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