

trans-2-Pentenoic acid

Other names:	(2E)-2-Pentenoic acid (E)-2-Pentenoic acid (E)-pent-2-en-1-oic acid 2-Pentenoic acid, (E)- trans-Alpha,beta-penteneoic acid
Inchi:	InChI=1S/C5H8O2/c1-2-3-4-5(6)7/h3-4H,2H2,1H3,(H,6,7)/b4-3+
InchiKey:	YIYBQIKDCADOSF-ONEGZZNKSA-N
Formula:	C5H8O2
SMILES:	CCC=CC(=O)O
Mol. weight [g/mol]:	100.12
CAS:	13991-37-2

Physical Properties

Property code	Value	Unit	Source
affp	823.60	kJ/mol	NIST Webbook
basg	792.60	kJ/mol	NIST Webbook
chl	-4020.00	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	4350.56 ± 100.00	kPa	NIST Webbook
tb	464.01	K	Joback Method
tc	676.92 ± 3.00	K	NIST Webbook
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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45186e+01
Coeff. B	-3.48091e+03
Coeff. C	-1.15948e+02
Temperature range (K), min.	360.55
Temperature range (K), max.	494.02

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13991372&Units=SI>

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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