

# Propanedioic acid, propyl-

<b>Other names:</b>	n-Propylmalonic acid
<b>Inchi:</b>	InChI=1S/C6H10O4/c1-2-3-4(5(7)8)6(9)10/h4H,2-3H2,1H3,(H,7,8)(H,9,10)
<b>InchiKey:</b>	VQDJODAWOFNASI-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O4
<b>SMILES:</b>	CCCC(C(=O)O)C(=O)O
<b>Mol. weight [g/mol]:</b>	146.14
<b>CAS:</b>	616-62-6

## Physical Properties

Property code	Value	Unit	Source
chs	-2827.20	kJ/mol	NIST Webbook
gf	-534.28	kJ/mol	Joback Method
hf	-702.07	kJ/mol	Joback Method
hfus	19.15	kJ/mol	Joback Method
hvap	75.41	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.572		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	628.34	K	Joback Method
tc	804.84	K	Joback Method
tf	369.00 ± 2.00	K	NIST Webbook
vc	0.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.07	J/mol×K	628.34	Joback Method
cpg	310.49	J/mol×K	775.42	Joback Method
cpg	304.69	J/mol×K	746.00	Joback Method
cpg	298.55	J/mol×K	716.59	Joback Method
cpg	292.08	J/mol×K	687.17	Joback Method
cpg	285.25	J/mol×K	657.76	Joback Method
cpg	315.96	J/mol×K	804.84	Joback Method

dvisc	0.0000353	Paxs	628.34	Joback Method
dvisc	0.0000632	Paxs	584.26	Joback Method
dvisc	0.0001243	Paxs	540.19	Joback Method
dvisc	0.0002758	Paxs	496.11	Joback Method
dvisc	0.0007147	Paxs	452.03	Joback Method
dvisc	0.0022752	Paxs	407.96	Joback Method
dvisc	0.0095884	Paxs	363.88	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.98753e+01
Coeff. B	-7.24164e+03
Coeff. C	-1.09896e+02
Temperature range (K), min.	479.60
Temperature range (K), max.	607.13

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C616626&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C616626&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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