

# Heptanoic acid, 2-ethyl-

<b>Other names:</b>	2-Ethylheptanoic acid 3-Octanecarboxylic acid
<b>Inchi:</b>	InChI=1S/C9H18O2/c1-3-5-6-7-8(4-2)9(10)11/h8H,3-7H2,1-2H3,(H,10,11)
<b>InchiKey:</b>	DYWSVUBJGFTOQC-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2
<b>SMILES:</b>	CCCCCC(CC)C(=O)O
<b>Mol. weight [g/mol]:</b>	158.24
<b>CAS:</b>	3274-29-1

## Physical Properties

Property code	Value	Unit	Source
gf	-243.28	kJ/mol	Joback Method
hf	-499.18	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.678		Crippen Method
mvol	145.110	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	550.93	K	Joback Method
tc	721.77	K	Joback Method
tf	286.94	K	Joback Method
vc	0.558	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.88	J/molxK	721.77	Joback Method
cpg	410.35	J/molxK	693.29	Joback Method
cpg	400.35	J/molxK	664.82	Joback Method
cpg	389.89	J/molxK	636.35	Joback Method
cpg	378.95	J/molxK	607.88	Joback Method
cpg	367.51	J/molxK	579.40	Joback Method
cpg	355.57	J/molxK	550.93	Joback Method

dvisc	0.0229838	Paxs	286.94	Joback Method
dvisc	0.0001171	Paxs	550.93	Joback Method
dvisc	0.0001927	Paxs	506.93	Joback Method
dvisc	0.0003486	Paxs	462.93	Joback Method
dvisc	0.0007142	Paxs	418.94	Joback Method
dvisc	0.0017314	Paxs	374.94	Joback Method
dvisc	0.0053119	Paxs	330.94	Joback Method
hvapt	63.40	kJ/mol	430.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54818e+01
Coeff. B	-4.72238e+03
Coeff. C	-8.49180e+01
Temperature range (K), min.	395.72
Temperature range (K), max.	549.25

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3274291&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3274291&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>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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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