

# 3,6-Heptanedione

<b>Other names:</b>	Heptane-2,5-dione
<b>Inchi:</b>	InChI=1S/C7H12O2/c1-3-7(9)5-4-6(2)8/h3-5H2,1-2H3
<b>InchiKey:</b>	HGRGPAAXHOTBAM-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O2
<b>SMILES:</b>	CCC(=O)CCC(C)=O
<b>Mol. weight [g/mol]:</b>	128.17
<b>CAS:</b>	1703-51-1

## Physical Properties

Property code	Value	Unit	Source
gf	-249.78	kJ/mol	Joback Method
hf	-412.97	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.335		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	163.30		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	163.30		NIST Webbook
tb	467.30	K	Joback Method
tc	655.05	K	Joback Method
tf	268.51	K	Joback Method
vc	0.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.34	J/mol×K	467.30	Joback Method
cpg	244.05	J/mol×K	498.59	Joback Method
cpg	254.28	J/mol×K	529.88	Joback Method

cpg	264.05	J/molxK	561.18	Joback Method
cpg	273.38	J/molxK	592.47	Joback Method
cpg	282.27	J/molxK	623.76	Joback Method
cpg	290.73	J/molxK	655.05	Joback Method
dvisc	0.0035564	Paxs	268.51	Joback Method
dvisc	0.0019557	Paxs	301.64	Joback Method
dvisc	0.0012106	Paxs	334.77	Joback Method
dvisc	0.0008169	Paxs	367.90	Joback Method
dvisc	0.0005883	Paxs	401.04	Joback Method
dvisc	0.0004455	Paxs	434.17	Joback Method
dvisc	0.0003508	Paxs	467.30	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1703511&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1703511&amp;Units=SI</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>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>rinpol:</b>	Non-polar retention indices
<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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