

# 3-methylhexane-2,5-dione

<b>Inchi:</b>	InChI=1S/C7H12O2/c1-5(7(3)9)4-6(2)8/h5H,4H2,1-3H3
<b>InchiKey:</b>	NLLILAUVOOREKR-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O2
<b>SMILES:</b>	CC(=O)CC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	128.17
<b>CAS:</b>	4437-50-7

## Physical Properties

Property code	Value	Unit	Source
gf	-252.22	kJ/mol	Joback Method
hf	-418.25	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.191		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	466.86	K	Joback Method
tc	658.82	K	Joback Method
tf	253.51	K	Joback Method
vc	0.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.52	J/mol×K	466.86	Joback Method
cpg	244.55	J/mol×K	498.85	Joback Method
cpg	255.07	J/mol×K	530.85	Joback Method
cpg	265.11	J/mol×K	562.84	Joback Method
cpg	274.67	J/mol×K	594.83	Joback Method
cpg	283.77	J/mol×K	626.83	Joback Method
cpg	292.41	J/mol×K	658.82	Joback Method
dvisc	0.0049833	Paxs	253.51	Joback Method
dvisc	0.0024070	Paxs	289.07	Joback Method

dvisc	0.0013635	Paxs	324.63	Joback Method
dvisc	0.0008641	Paxs	360.19	Joback Method
dvisc	0.0005944	Paxs	395.74	Joback Method
dvisc	0.0004349	Paxs	431.30	Joback Method
dvisc	0.0003337	Paxs	466.86	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4437507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4437507&amp;Units=SI</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>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>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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