

# Heptacosane-2,4-dione

<b>Inchi:</b>	InChI=1S/C27H52O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27
<b>InchiKey:</b>	YAMQASNSNZBZPD-UHFFFAOYSA-N
<b>Formula:</b>	C27H52O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
<b>Mol. weight [g/mol]:</b>	408.70
<b>CAS:</b>	112468-39-0

## Physical Properties

Property code	Value	Unit	Source
gf	-81.38	kJ/mol	Joback Method
hf	-825.77	kJ/mol	Joback Method
hfus	68.88	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-9.68		Crippen Method
logp	9.137		Crippen Method
mcvol	394.430	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	3028.50		NIST Webbook
rinpol	3028.50		NIST Webbook
tb	924.90	K	Joback Method
tc	1136.76	K	Joback Method
tf	493.91	K	Joback Method
vc	1.560	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.12	J/molxK	924.90	Joback Method
cpg	1443.36	J/molxK	1101.45	Joback Method
cpg	1426.03	J/molxK	1066.14	Joback Method
cpg	1407.51	J/molxK	1030.83	Joback Method
cpg	1387.74	J/molxK	995.52	Joback Method
cpg	1366.64	J/molxK	960.21	Joback Method
cpg	1459.59	J/molxK	1136.76	Joback Method

dvisc	0.0000341	Paxs	924.90	Joback Method
dvisc	0.0000462	Paxs	853.07	Joback Method
dvisc	0.0000662	Paxs	781.24	Joback Method
dvisc	0.0001022	Paxs	709.40	Joback Method
dvisc	0.0001739	Paxs	637.57	Joback Method
dvisc	0.0003384	Paxs	565.74	Joback Method
dvisc	0.0007997	Paxs	493.91	Joback Method

## Sources

<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=C112468390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C112468390&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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>mvol:</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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