

# Malonic acid, 4-heptyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C25H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-28-24(26)22-25(27)29-
<b>InchiKey:</b>	PIDZOGWEHKUPHP-UHFFFAOYSA-N
<b>Formula:</b>	C25H48O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CC(=O)OC(CCC)CCC
<b>Mol. weight [g/mol]:</b>	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	-310.66	kJ/mol	Joback Method
hf	-1054.21	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.523		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpola	2694.00		NIST Webbook
tb	923.54	K	Joback Method
tc	1133.47	K	Joback Method
tf	500.83	K	Joback Method
vc	1.478	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.56	J/molxK	923.54	Joback Method
cpg	1302.20	J/molxK	958.53	Joback Method
cpg	1321.30	J/molxK	993.52	Joback Method
cpg	1338.92	J/molxK	1028.50	Joback Method
cpg	1355.09	J/molxK	1063.49	Joback Method
cpg	1369.84	J/molxK	1098.48	Joback Method
cpg	1383.23	J/molxK	1133.47	Joback Method
dvisc	0.0005334	Paxs	500.83	Joback Method
dvisc	0.0002287	Paxs	571.28	Joback Method

dvisc	0.0001181	Paxs	641.73	Joback Method
dvisc	0.0000695	Paxs	712.18	Joback Method
dvisc	0.0000450	Paxs	782.64	Joback Method
dvisc	0.0000313	Paxs	853.09	Joback Method
dvisc	0.0000230	Paxs	923.54	Joback Method

## Sources

<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=U349000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349000&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>

## 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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