

# Malonic acid, hexadecyl 3-methylpent-2-yl ester

Inchi:	InChI=1S/C25H48O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-28-24(26)21-25(27)
InchiKey:	GZCZYSAIINNLEF-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	-313.10	kJ/mol	Joback Method
hf	-1059.49	kJ/mol	Joback Method
hfus	59.03	kJ/mol	Joback Method
hvap	88.78	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.379		Crippen Method
mvol	377.990	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	923.10	K	Joback Method
tc	1132.09	K	Joback Method
tf	485.83	K	Joback Method
vc	1.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.95	J/molxK	923.10	Joback Method
cpg	1302.47	J/molxK	957.93	Joback Method
cpg	1321.46	J/molxK	992.76	Joback Method
cpg	1338.96	J/molxK	1027.60	Joback Method
cpg	1355.01	J/molxK	1062.43	Joback Method
cpg	1369.65	J/molxK	1097.26	Joback Method
cpg	1382.92	J/molxK	1132.09	Joback Method
dvisc	0.0006234	Paxs	485.83	Joback Method

dvisc	0.0002451	Paxs	558.71	Joback Method
dvisc	0.0001196	Paxs	631.59	Joback Method
dvisc	0.0000676	Paxs	704.47	Joback Method
dvisc	0.0000426	Paxs	777.34	Joback Method
dvisc	0.0000290	Paxs	850.22	Joback Method
dvisc	0.0000210	Paxs	923.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349317&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349317&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>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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