

# 1,2,3-Propanetricarboxylic acid, 2-acetoxy-, tri-(2-methylpentyl) ester

Inchi:	InChI=1S/C26H46O8/c1-8-11-19(4)16-31-23(28)14-26(34-22(7)27,25(30)33-18-21(6)13-
InchiKey:	LYBREHQJEADDPS-UHFFFAOYSA-N
Formula:	C26H46O8
SMILES:	CCCC(C)COC(=O)CC(CC(=O)OCC(C)CCC)(OC(C)=O)C(=O)OCC(C)CCC
Mol. weight [g/mol]:	486.64

## Physical Properties

Property code	Value	Unit	Source
gf	-772.12	kJ/mol	Joback Method
hf	-1583.76	kJ/mol	Joback Method
hfus	56.26	kJ/mol	Joback Method
hvap	107.63	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.007		Crippen Method
mcvol	406.960	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
tb	1094.89	K	Joback Method
tc	1356.80	K	Joback Method
tf	628.84	K	Joback Method
vc	1.558	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.64	J/molxK	1094.89	Joback Method
cpg	1447.78	J/molxK	1138.54	Joback Method
cpg	1459.39	J/molxK	1182.19	Joback Method
cpg	1468.52	J/molxK	1225.84	Joback Method
cpg	1475.21	J/molxK	1269.50	Joback Method
cpg	1479.54	J/molxK	1313.15	Joback Method
cpg	1481.55	J/molxK	1356.80	Joback Method
dvisc	0.0001210	Paxs	628.84	Joback Method
dvisc	0.0000543	Paxs	706.51	Joback Method
dvisc	0.0000285	Paxs	784.19	Joback Method

dvisc	0.0000168	Paxs	861.87	Joback Method
dvisc	0.0000108	Paxs	939.54	Joback Method
dvisc	0.0000075	Paxs	1017.21	Joback Method
dvisc	0.0000054	Paxs	1094.89	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=B6009469&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009469&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>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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