

# 1,3,5-Cyclohexanetriol, 2,2,4,4,6,6-hexamethyl-, tripelargonate

<b>Inchi:</b>	InChI=1S/C39H72O6/c1-10-13-16-19-22-25-28-31(40)43-34-37(4,5)35(44-32(41)29-26-2
<b>InchiKey:</b>	ZIZJJUPWGPVRKO-UHFFFAOYSA-N
<b>Formula:</b>	C39H72O6
<b>SMILES:</b>	CCCCCCCC(=O)OC1C(C)(C)C(OC(=O)CCCCCCCC)C(C)(C)C(OC(=O)CCCCCCCC)C
<b>Mol. weight [g/mol]:</b>	636.99

## Physical Properties

Property code	Value	Unit	Source
gf	-454.83	kJ/mol	Joback Method
hf	-1584.35	kJ/mol	Joback Method
hfus	83.42	kJ/mol	Joback Method
hvap	125.31	kJ/mol	Joback Method
log10ws	-12.24		Crippen Method
logp	11.066		Crippen Method
mcvol	571.830	ml/mol	McGowan Method
pc	462.68	kPa	Joback Method
tb	1317.51	K	Joback Method
tc	1752.40	K	Joback Method
tf	803.65	K	Joback Method
vc	2.213	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2488.83	J/molxK	1317.51	Joback Method
cpg	2598.29	J/molxK	1389.99	Joback Method
cpg	2719.92	J/molxK	1462.47	Joback Method
cpg	2856.08	J/molxK	1534.95	Joback Method
cpg	3009.10	J/molxK	1607.44	Joback Method
cpg	3181.33	J/molxK	1679.92	Joback Method
cpg	3375.09	J/molxK	1752.40	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=B6000775&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000775&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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