

# Ethylene glycol bis(2,2,4-trimethyl-3-oxovalerate)

**Inchi:** InChI=1S/C18H30O6/c1-11(2)13(19)17(5,6)15(21)23-9-10-24-16(22)18(7,8)14(20)12(3)4

**InchiKey:** BEGGHCFDNUXHDL-UHFFFAOYSA-N

**Formula:** C18H30O6

**SMILES:** CC(C)C(=O)C(C)(C)C(=O)OCCOC(=O)C(C)(C)C(=O)C(C)C

**Mol. weight [g/mol]:** 342.43

**CAS:** 4447-67-0

## Physical Properties

Property code	Value	Unit	Source
gf	-624.20	kJ/mol	Joback Method
hf	-1157.67	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.575		Crippen Method
mcvol	282.500	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
tb	864.22	K	Joback Method
tc	1071.19	K	Joback Method
tf	511.64	K	Joback Method
vc	1.069	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.32	J/molxK	864.22	Joback Method
cpg	908.05	J/molxK	898.71	Joback Method
cpg	921.67	J/molxK	933.21	Joback Method
cpg	934.22	J/molxK	967.70	Joback Method
cpg	945.76	J/molxK	1002.20	Joback Method
cpg	956.32	J/molxK	1036.69	Joback Method
cpg	965.97	J/molxK	1071.19	Joback Method
dvisc	0.0006820	Paxs	511.64	Joback Method
dvisc	0.0003179	Paxs	570.40	Joback Method

dvisc	0.0001709	Paxs	629.17	Joback Method
dvisc	0.0001021	Paxs	687.93	Joback Method
dvisc	0.0000662	Paxs	746.69	Joback Method
dvisc	0.0000457	Paxs	805.46	Joback Method
dvisc	0.0000332	Paxs	864.22	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=C4447670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4447670&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>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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