

# Propylene glycol monobutyrate (s)

<b>Inchi:</b>	InChI=1S/C7H14O3/c1-3-4-7(9)10-6(2)5-8/h6,8H,3-5H2,1-2H3
<b>InchiKey:</b>	RNNACNWQHUTWGB-UHFFFAOYSA-N
<b>Formula:</b>	C7H14O3
<b>SMILES:</b>	CCCC(=O)OC(C)CO
<b>Mol. weight [g/mol]:</b>	146.18

## Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-590.12	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinsol	1028.00		NIST Webbook
tb	527.59	K	Joback Method
tc	700.51	K	Joback Method
tf	286.63	K	Joback Method
vc	0.465	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/molxK	527.59	Joback Method
cpg	298.85	J/molxK	556.41	Joback Method
cpg	308.56	J/molxK	585.23	Joback Method
cpg	317.88	J/molxK	614.05	Joback Method
cpg	326.83	J/molxK	642.87	Joback Method
cpg	335.40	J/molxK	671.69	Joback Method
cpg	343.59	J/molxK	700.51	Joback Method
dvisc	0.0172601	Paxs	286.63	Joback Method
dvisc	0.0045782	Paxs	326.79	Joback Method

dvisc	0.0016237	Paxs	366.95	Joback Method
dvisc	0.0007065	Paxs	407.11	Joback Method
dvisc	0.0003570	Paxs	447.27	Joback Method
dvisc	0.0002019	Paxs	487.43	Joback Method
dvisc	0.0001245	Paxs	527.59	Joback Method

## Sources

<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=R543692&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R543692&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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