

# Butane-2,3-diol, mono-hexanoate, #2

<b>Inchi:</b>	InChI=1S/C12H24O3/c1-6-7-8-9-10(13)15-12(4,5)11(2,3)14/h14H,6-9H2,1-5H3
<b>InchiKey:</b>	XGWLQGQNKWAYLA-UHFFFAOYSA-N
<b>Formula:</b>	C12H24O3
<b>SMILES:</b>	CCCCCC(=O)OC(C)(C)C(C)(C)O
<b>Mol. weight [g/mol]:</b>	216.32

## Physical Properties

Property code	Value	Unit	Source
gf	-314.90	kJ/mol	Joback Method
hf	-705.54	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.659		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1282.00		NIST Webbook
tb	635.97	K	Joback Method
tc	816.26	K	Joback Method
tf	362.82	K	Joback Method
vc	0.729	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.03	J/molxK	635.97	Joback Method
cpg	550.53	J/molxK	666.02	Joback Method
cpg	564.26	J/molxK	696.07	Joback Method
cpg	577.25	J/molxK	726.11	Joback Method
cpg	589.53	J/molxK	756.16	Joback Method
cpg	601.13	J/molxK	786.21	Joback Method
cpg	612.11	J/molxK	816.26	Joback Method

dvisc	0.0047728	Paxs	362.82	Joback Method
dvisc	0.0013923	Paxs	408.35	Joback Method
dvisc	0.0005200	Paxs	453.87	Joback Method
dvisc	0.0002324	Paxs	499.39	Joback Method
dvisc	0.0001189	Paxs	544.92	Joback Method
dvisc	0.0000674	Paxs	590.45	Joback Method
dvisc	0.0000415	Paxs	635.97	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=R66344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R66344&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>mvol:</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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