

# butyl 6-methyloctanoate

<b>Inchi:</b>	InChI=1S/C13H26O2/c1-4-6-11-15-13(14)10-8-7-9-12(3)5-2/h12H,4-11H2,1-3H3
<b>InchiKey:</b>	NDJNECCQUKGLOH-UHFFFAOYSA-N
<b>Formula:</b>	C13H26O2
<b>SMILES:</b>	CCCCOC(=O)CCCC(C)CC
<b>Mol. weight [g/mol]:</b>	214.34

## Physical Properties

Property code	Value	Unit	Source
gf	-177.78	kJ/mol	Joback Method
hf	-561.73	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.936		Crippen Method
mvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
ripol	1667.00		NIST Webbook
ripol	1667.00		NIST Webbook
tb	572.69	K	Joback Method
tc	744.36	K	Joback Method
tf	293.43	K	Joback Method
vc	0.781	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/molxK	572.69	Joback Method
cpg	591.64	J/molxK	715.75	Joback Method
cpg	577.64	J/molxK	687.14	Joback Method
cpg	563.00	J/molxK	658.53	Joback Method
cpg	547.70	J/molxK	629.91	Joback Method
cpg	531.74	J/molxK	601.30	Joback Method
cpg	605.00	J/molxK	744.36	Joback Method
dvisc	0.0001594	Paxs	572.69	Joback Method

dvisc	0.0002152	Paxs	526.15	Joback Method
dvisc	0.0003078	Paxs	479.60	Joback Method
dvisc	0.0004755	Paxs	433.06	Joback Method
dvisc	0.0008156	Paxs	386.52	Joback Method
dvisc	0.0016218	Paxs	339.97	Joback Method
dvisc	0.0040106	Paxs	293.43	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R493364&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R493364&amp;Units=SI</a>
<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>

## 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>ripol:</b>	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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