

# 5-Bromovaleric acid, tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C18H31BrO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-21-18(20)15-12-13-16-19/h2-10,
<b>InchiKey:</b>	JUXZXAPWMXWRKX-UHFFFAOYSA-N
<b>Formula:</b>	C18H31BrO2
<b>SMILES:</b>	CCCCCCCCCCC#CCOC(=O)CCCCBr
<b>Mol. weight [g/mol]:</b>	359.34

## Physical Properties

Property code	Value	Unit	Source
gf	83.88	kJ/mol	Joback Method
hf	-361.02	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.629		Crippen Method
mvol	280.820	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2367.10		NIST Webbook
rinpol	2367.10		NIST Webbook
tb	762.69	K	Joback Method
tc	954.00	K	Joback Method
tf	530.68	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.87	J/mol×K	762.69	Joback Method
cpg	813.91	J/mol×K	794.58	Joback Method
cpg	830.06	J/mol×K	826.46	Joback Method
cpg	845.33	J/mol×K	858.35	Joback Method
cpg	859.76	J/mol×K	890.23	Joback Method
cpg	873.38	J/mol×K	922.12	Joback Method
cpg	886.22	J/mol×K	954.00	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=U292570&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292570&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>

# 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>hvp:</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>rinp:</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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