

# 2-Bromobenzoic acid, 2-methyloct-5-yn-4-yl ester

<b>Inchi:</b>	InChI=1S/C16H19BrO2/c1-4-5-8-13(11-12(2)3)19-16(18)14-9-6-7-10-15(14)17/h6-7,9-10
<b>InchiKey:</b>	NZYBMUABIJRVEC-UHFFFAOYSA-N
<b>Formula:</b>	C16H19BrO2
<b>SMILES:</b>	CCC#CC(CC(C)C)OC(=O)c1ccccc1Br
<b>Mol. weight [g/mol]:</b>	323.23

## Physical Properties

Property code	Value	Unit	Source
gf	164.94	kJ/mol	Joback Method
hf	-105.24	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.434		Crippen Method
mcvol	228.880	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpola	1951.00		NIST Webbook
tb	747.71	K	Joback Method
tc	982.45	K	Joback Method
tf	517.08	K	Joback Method
vc	0.860	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.87	J/mol×K	747.71	Joback Method
cpg	613.43	J/mol×K	786.83	Joback Method
cpg	627.86	J/mol×K	825.96	Joback Method
cpg	641.23	J/mol×K	865.08	Joback Method
cpg	653.57	J/mol×K	904.21	Joback Method
cpg	664.94	J/mol×K	943.33	Joback Method
cpg	675.37	J/mol×K	982.45	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299396&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>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>mccvol:</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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