

# 6-Bromohexanoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C17H27BrO2/c1-5-9-15(4)16(12-11-14(2)3)20-17(19)10-7-6-8-13-18/h15-16H,

InchiKey: MARGMJPGEDHQB-UHFFFAOYSA-N

Formula: C17H27BrO2

SMILES: C=C(C)C#CC(OC(=O)CCCCCBr)C(C)CCC

Mol. weight [g/mol]: 343.30

## Physical Properties

Property code	Value	Unit	Source
gf	149.87	kJ/mol	Joback Method
hf	-235.30	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.869		Crippen Method
mvol	262.430	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	735.49	K	Joback Method
tc	937.64	K	Joback Method
tf	473.69	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.36	J/mol×K	735.49	Joback Method
cpg	732.21	J/mol×K	769.18	Joback Method
cpg	748.12	J/mol×K	802.87	Joback Method
cpg	763.11	J/mol×K	836.56	Joback Method
cpg	777.23	J/mol×K	870.26	Joback Method
cpg	790.52	J/mol×K	903.95	Joback Method
cpg	803.01	J/mol×K	937.64	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=U299293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299293&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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