

# Bromoacetic acid, octyl ester

<b>Other names:</b>	Octyl bromoacetate
<b>Inchi:</b>	InChI=1S/C10H19BrO2/c1-2-3-4-5-6-7-8-13-10(12)9-11/h2-9H2,1H3
<b>InchiKey:</b>	ZBNUZMDEFBLZIJ-UHFFFAOYSA-N
<b>Formula:</b>	C10H19BrO2
<b>SMILES:</b>	CCCCCCCCOC(=O)CBr
<b>Mol. weight [g/mol]:</b>	251.16
<b>CAS:</b>	38674-98-5

## Physical Properties

Property code	Value	Unit	Source
gf	-186.28	kJ/mol	Joback Method
hf	-468.20	kJ/mol	Joback Method
hfus	29.73	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.285		Crippen Method
mcvol	176.700	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1484.10		NIST Webbook
tb	570.65	K	Joback Method
tc	756.07	K	Joback Method
tf	334.42	K	Joback Method
vc	0.681	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.99	J/molxK	570.65	Joback Method
cpg	426.59	J/molxK	601.55	Joback Method
cpg	439.57	J/molxK	632.46	Joback Method
cpg	451.95	J/molxK	663.36	Joback Method
cpg	463.74	J/molxK	694.27	Joback Method
cpg	474.96	J/molxK	725.17	Joback Method
cpg	485.63	J/molxK	756.07	Joback Method

dvisc	0.0023247	Paxs	334.42	Joback Method
dvisc	0.0012758	Paxs	373.79	Joback Method
dvisc	0.0007850	Paxs	413.16	Joback Method
dvisc	0.0005256	Paxs	452.53	Joback Method
dvisc	0.0003752	Paxs	491.91	Joback Method
dvisc	0.0002816	Paxs	531.28	Joback Method
dvisc	0.0002199	Paxs	570.65	Joback Method

## Sources

<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=C38674985&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38674985&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.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>

## 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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