

# Butanoic acid, 2,3-dibromo-, ethyl ester

<b>Other names:</b>	Butyric acid, 2,3-dibromo-, ethyl ester Ethyl 2,3-dibromobutanoate Ethyl 2,3-dibromobutyrate Ethyl «alpha», «beta»-dibromobutyrate
<b>Inchi:</b>	InChI=1S/C6H10Br2O2/c1-3-10-6(9)5(8)4(2)7/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	YPZLAXFGOUPECS-UHFFFAOYSA-N
<b>Formula:</b>	C6H10Br2O2
<b>SMILES:</b>	CCOC(=O)C(Br)C(C)Br
<b>Mol. weight [g/mol]:</b>	273.95
<b>CAS:</b>	609-11-0

## Physical Properties

Property code	Value	Unit	Source
gf	-210.52	kJ/mol	Joback Method
hf	-369.87	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.096		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	544.41	K	Joback Method
tc	762.87	K	Joback Method
tf	319.14	K	Joback Method
vc	0.507	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.87	J/molxK	544.41	Joback Method
cpg	278.66	J/molxK	580.82	Joback Method
cpg	287.88	J/molxK	617.23	Joback Method
cpg	296.57	J/molxK	653.64	Joback Method
cpg	304.73	J/molxK	690.05	Joback Method

cpg	312.38	J/mol×K	726.46	Joback Method
cpg	319.55	J/mol×K	762.87	Joback Method
dvisc	0.0031975	Paxs	319.14	Joback Method
dvisc	0.0017149	Paxs	356.69	Joback Method
dvisc	0.0010356	Paxs	394.23	Joback Method
dvisc	0.0006828	Paxs	431.77	Joback Method
dvisc	0.0004812	Paxs	469.32	Joback Method
dvisc	0.0003571	Paxs	506.86	Joback Method
dvisc	0.0002762	Paxs	544.41	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=C609110&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C609110&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>

## 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>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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