

# 4-Bromobutyric acid, 4-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C10H10BrClO2/c11-7-1-2-10(13)14-9-5-3-8(12)4-6-9/h3-6H,1-2,7H2
<b>InchiKey:</b>	SFZQUTXYCIPZCO-UHFFFAOYSA-N
<b>Formula:</b>	C10H10BrClO2
<b>SMILES:</b>	O=C(CCCBr)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	277.54

## Physical Properties

Property code	Value	Unit	Source
gf	-95.43	kJ/mol	Joback Method
hf	-258.88	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.421		Crippen Method
mcvol	165.180	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	639.74	K	Joback Method
tc	870.25	K	Joback Method
tf	403.28	K	Joback Method
vc	0.623	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.45	J/molxK	639.74	Joback Method
cpg	371.79	J/molxK	678.16	Joback Method
cpg	382.33	J/molxK	716.58	Joback Method
cpg	392.11	J/molxK	754.99	Joback Method
cpg	401.16	J/molxK	793.41	Joback Method
cpg	409.51	J/molxK	831.83	Joback Method
cpg	417.18	J/molxK	870.25	Joback Method
dvisc	0.0013065	Paxs	403.28	Joback Method

dvisc	0.0008294	Paxs	442.69	Joback Method
dvisc	0.0005671	Paxs	482.10	Joback Method
dvisc	0.0004107	Paxs	521.51	Joback Method
dvisc	0.0003112	Paxs	560.92	Joback Method
dvisc	0.0002446	Paxs	600.33	Joback Method
dvisc	0.0001980	Paxs	639.74	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307607&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307607&amp;Units=SI</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>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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