

# Hexyl 2-bromobutanoate

<b>Inchi:</b>	InChI=1S/C10H19BrO2/c1-3-5-6-7-8-13-10(12)9(11)4-2/h9H,3-8H2,1-2H3
<b>InchiKey:</b>	AXPPUDLSKDAEGB-UHFFFAOYSA-N
<b>Formula:</b>	C10H19BrO2
<b>SMILES:</b>	CCCCCCOC(=O)C(Br)CC
<b>Mol. weight [g/mol]:</b>	251.16

## Physical Properties

Property code	Value	Unit	Source
gf	-188.72	kJ/mol	Joback Method
hf	-473.48	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.283		Crippen Method
mcvol	176.700	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	570.21	K	Joback Method
tc	759.20	K	Joback Method
tf	319.42	K	Joback Method
vc	0.675	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.36	J/molxK	570.21	Joback Method
cpg	427.26	J/molxK	601.71	Joback Method
cpg	440.53	J/molxK	633.21	Joback Method
cpg	453.16	J/molxK	664.71	Joback Method
cpg	465.18	J/molxK	696.20	Joback Method
cpg	476.60	J/molxK	727.70	Joback Method
cpg	487.43	J/molxK	759.20	Joback Method
dvisc	0.0029907	Paxs	319.42	Joback Method

dvisc	0.0014794	Paxs	361.22	Joback Method
dvisc	0.0008469	Paxs	403.02	Joback Method
dvisc	0.0005384	Paxs	444.82	Joback Method
dvisc	0.0003699	Paxs	486.61	Joback Method
dvisc	0.0002698	Paxs	528.41	Joback Method
dvisc	0.0002060	Paxs	570.21	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=R23184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R23184&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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