

# dl-3,4-dibromohexane

<b>Inchi:</b>	InChI=1S/C6H12Br2/c1-3-5(7)6(8)4-2/h5-6H,3-4H2,1-2H3
<b>InchiKey:</b>	VCQBYNRFLHNSKA-UHFFFAOYSA-N
<b>Formula:</b>	C6H12Br2
<b>SMILES:</b>	CCC(Br)C(Br)CC
<b>Mol. weight [g/mol]:</b>	243.97

## Physical Properties

Property code	Value	Unit	Source
gf	23.40	kJ/mol	Joback Method
hf	-125.07	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.333		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
tb	468.12	K	Joback Method
tc	679.14	K	Joback Method
tf	246.98	K	Joback Method
vc	0.483	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.43	J/mol×K	468.12	Joback Method
cpg	245.45	J/mol×K	503.29	Joback Method
cpg	255.83	J/mol×K	538.46	Joback Method
cpg	265.60	J/mol×K	573.63	Joback Method
cpg	274.79	J/mol×K	608.80	Joback Method
cpg	283.45	J/mol×K	643.97	Joback Method
cpg	291.59	J/mol×K	679.14	Joback Method
dvisc	0.0061816	Paxs	246.98	Joback Method

dvisc	0.0027790	Paxs	283.84	Joback Method
dvisc	0.0015014	Paxs	320.69	Joback Method
dvisc	0.0009209	Paxs	357.55	Joback Method
dvisc	0.0006189	Paxs	394.41	Joback Method
dvisc	0.0004452	Paxs	431.26	Joback Method
dvisc	0.0003373	Paxs	468.12	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R244127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R244127&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>
<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>

## 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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