

# trans-1,2-Dibromocycloheptane

Inchi:	InChI=1S/C7H12Br2/c8-6-4-2-1-3-5-7(6)9/h6-7H,1-5H2/t6-,7+
InchiKey:	PQKOJNVKGNOTKZ-KNVOCYPGSA-N
Formula:	C7H12Br2
SMILES:	BrC1CCCCC1Br
Mol. weight [g/mol]:	255.98
CAS:	52021-35-9

## Physical Properties

Property code	Value	Unit	Source
gf	41.34	kJ/mol	Joback Method
hf	-107.33	kJ/mol	Joback Method
hfus	15.26	kJ/mol	Joback Method
hvap	52.02	kJ/mol	NIST Webbook
log10ws	-3.73		Crippen Method
logp	3.478		Crippen Method
mvol	133.630	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	511.03	K	Joback Method
tc	761.30	K	Joback Method
tf	287.87	K	Joback Method
vc	0.475	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.05	J/molxK	511.03	Joback Method
cpg	332.42	J/molxK	719.58	Joback Method
cpg	320.06	J/molxK	677.87	Joback Method
cpg	306.68	J/molxK	636.16	Joback Method
cpg	292.25	J/molxK	594.45	Joback Method
cpg	276.72	J/molxK	552.74	Joback Method
cpg	343.80	J/molxK	761.30	Joback Method
dvisc	0.0003245	Paxs	511.03	Joback Method
dvisc	0.0004168	Paxs	473.84	Joback Method

dvisc	0.0005586	Paxs	436.64	Joback Method
dvisc	0.0007907	Paxs	399.45	Joback Method
dvisc	0.0012019	Paxs	362.26	Joback Method
dvisc	0.0020105	Paxs	325.06	Joback Method
dvisc	0.0038417	Paxs	287.87	Joback Method

## Sources

<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=C52021359&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52021359&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>

## 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>mccvol:</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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