

# Propanone, pentabromo-

<b>Inchi:</b>	InChI=1S/C3HBr5O/c4-2(5)1(9)3(6,7)8/h2H
<b>InchiKey:</b>	OEQPNRAFDGLBAW-UHFFFAOYSA-N
<b>Formula:</b>	C3HBr5O
<b>SMILES:</b>	O=C(C(Br)Br)C(Br)(Br)Br
<b>Mol. weight [g/mol]:</b>	452.56
<b>CAS:</b>	79-49-2

## Physical Properties

Property code	Value	Unit	Source
gf	-82.54	kJ/mol	Joback Method
hf	-100.21	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.510		Crippen Method
mcvol	142.200	ml/mol	McGowan Method
pc	8718.08	kPa	Joback Method
tb	649.04	K	Joback Method
tc	939.48	K	Joback Method
tf	459.92	K	Joback Method
vc	0.502	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.45	J/molxK	649.04	Joback Method
cpg	206.10	J/molxK	891.07	Joback Method
cpg	204.54	J/molxK	842.66	Joback Method
cpg	202.97	J/molxK	794.26	Joback Method
cpg	201.21	J/molxK	745.85	Joback Method
cpg	199.10	J/molxK	697.45	Joback Method
cpg	207.82	J/molxK	939.48	Joback Method
dvisc	0.0002699	Paxs	649.04	Joback Method
dvisc	0.0003296	Paxs	617.52	Joback Method

dvisc	0.0004113	Paxs	586.00	Joback Method
dvisc	0.0005262	Paxs	554.48	Joback Method
dvisc	0.0006937	Paxs	522.96	Joback Method
dvisc	0.0009474	Paxs	491.44	Joback Method
dvisc	0.0013503	Paxs	459.92	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C79492&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79492&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>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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