

# Heptane, 1-bromo-6-methyl-

<b>Other names:</b>	1-Bromo-6-methylheptane
<b>Inchi:</b>	InChI=1S/C8H17Br/c1-8(2)6-4-3-5-7-9/h8H,3-7H2,1-2H3
<b>InchiKey:</b>	BFYPQDKZLOZOLQ-UHFFFAOYSA-N
<b>Formula:</b>	C8H17Br
<b>SMILES:</b>	CC(C)CCCCCBr
<b>Mol. weight [g/mol]:</b>	193.12
<b>CAS:</b>	52648-04-1

## Physical Properties

Property code	Value	Unit	Source
gf	28.36	kJ/mol	Joback Method
hf	-187.40	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.598		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	448.16	K	Joback Method
tc	633.14	K	Joback Method
tf	224.72	K	Joback Method
vc	0.539	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.18	J/molxK	448.16	Joback Method
cpg	290.54	J/molxK	478.99	Joback Method
cpg	303.29	J/molxK	509.82	Joback Method
cpg	315.46	J/molxK	540.65	Joback Method
cpg	327.07	J/molxK	571.48	Joback Method
cpg	338.14	J/molxK	602.31	Joback Method
cpg	348.69	J/molxK	633.14	Joback Method
dvisc	0.0063866	Paxs	224.72	Joback Method

dvisc	0.0026570	Paxs	261.96	Joback Method
dvisc	0.0013751	Paxs	299.20	Joback Method
dvisc	0.0008234	Paxs	336.44	Joback Method
dvisc	0.0005461	Paxs	373.68	Joback Method
dvisc	0.0003902	Paxs	410.92	Joback Method
dvisc	0.0002948	Paxs	448.16	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53071e+01
Coeff. B	-4.22096e+03
Coeff. C	-7.01280e+01
Temperature range (K), min.	351.16
Temperature range (K), max.	492.41

## Sources

<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=C52648041&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52648041&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

## 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>pvap:</b>	Vapor 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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