

# Pentane, 2-bromo-

<b>Other names:</b>	2-Bromopentane 2-Pentyl bromide NSC 7896 UN 2343
<b>Inchi:</b>	InChI=1S/C5H11Br/c1-3-4-5(2)6/h5H,3-4H2,1-2H3
<b>InchiKey:</b>	LGAJYTCRJPCZRJ-UHFFFAOYSA-N
<b>Formula:</b>	C5H11Br
<b>SMILES:</b>	CCCC(C)Br
<b>Mol. weight [g/mol]:</b>	151.04
<b>CAS:</b>	107-81-3

## Physical Properties

Property code	Value	Unit	Source
gf	3.10	kJ/mol	Joback Method
hf	-125.48	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.570		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
ripol	786.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	984.00		NIST Webbook
ripol	976.00		NIST Webbook
ripol	986.00		NIST Webbook
tb	379.52	K	Joback Method
tc	568.83	K	Joback Method
tf	190.91	K	Joback Method
vc	0.371	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	212.94	J/molxK	568.83	Joback Method
cpg	205.34	J/molxK	537.28	Joback Method
cpg	197.35	J/molxK	505.73	Joback Method
cpg	188.97	J/molxK	474.18	Joback Method
cpg	180.18	J/molxK	442.62	Joback Method
cpg	170.96	J/molxK	411.07	Joback Method
cpg	161.30	J/molxK	379.52	Joback Method
dvisc	0.0061616	Paxs	190.91	Joback Method
dvisc	0.0003481	Paxs	379.52	Joback Method
dvisc	0.0004527	Paxs	348.08	Joback Method
dvisc	0.0006202	Paxs	316.65	Joback Method
dvisc	0.0009108	Paxs	285.21	Joback Method
dvisc	0.0014710	Paxs	253.78	Joback Method
dvisc	0.0027207	Paxs	222.34	Joback Method
hvapt	37.50	kJ/mol	367.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48220e+01
Coeff. B	-3.57127e+03
Coeff. C	-4.00030e+01
Temperature range (K), min.	285.71
Temperature range (K), max.	415.51

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107813&Units=SI>

**The Yaws Handbook of Vapor Pressure:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

# 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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