

# Pentane, 2,4-dibromo-, (R\*,R\*)-(±)-

<b>Inchi:</b>	InChI=1S/C5H10Br2/c1-4(6)3-5(2)7/h4-5H,3H2,1-2H3/t4-,5-/m0/s1
<b>InchiKey:</b>	KUZOHDYKJXNCSI-WHFBIAKZSA-N
<b>Formula:</b>	C5H10Br2
<b>SMILES:</b>	CC(Br)CC(C)Br
<b>Mol. weight [g/mol]:</b>	229.94
<b>CAS:</b>	1625-68-9

## Physical Properties

Property code	Value	Unit	Source
gf	14.98	kJ/mol	Joback Method
hf	-104.43	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	38.82	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.943		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	445.24	K	Joback Method
tc	659.19	K	Joback Method
tf	235.71	K	Joback Method
vc	0.427	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.24	J/molxK	445.24	Joback Method
cpg	204.99	J/molxK	480.90	Joback Method
cpg	214.15	J/molxK	516.56	Joback Method
cpg	222.76	J/molxK	552.22	Joback Method
cpg	230.84	J/molxK	587.88	Joback Method
cpg	238.42	J/molxK	623.54	Joback Method
cpg	245.55	J/molxK	659.19	Joback Method
dvisc	0.0063998	Paxs	235.71	Joback Method
dvisc	0.0029311	Paxs	270.63	Joback Method

dvisc	0.0016048	Paxs	305.55	Joback Method
dvisc	0.0009942	Paxs	340.48	Joback Method
dvisc	0.0006733	Paxs	375.40	Joback Method
dvisc	0.0004872	Paxs	410.32	Joback Method
dvisc	0.0003710	Paxs	445.24	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=C1625689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1625689&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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