

# Pentatriacontane, 1-bromo-

<b>Inchi:</b>	InChI=1S/C35H71Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24
<b>InchiKey:</b>	MEBUIUJNXZWZJQ-UHFFFAOYSA-N
<b>Formula:</b>	C35H71Br
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCBr
<b>Mol. weight [g/mol]:</b>	571.84
<b>CAS:</b>	62108-51-4

## Physical Properties

Property code	Value	Unit	Source
gf	258.14	kJ/mol	Joback Method
hf	-739.40	kJ/mol	Joback Method
hfus	91.69	kJ/mol	Joback Method
hvap	99.94	kJ/mol	Joback Method
log10ws	-14.90		Crippen Method
logp	14.274		Crippen Method
mcvol	521.510	ml/mol	McGowan Method
pc	491.86	kPa	Joback Method
tb	1066.36	K	Joback Method
tc	1364.24	K	Joback Method
tf	544.01	K	Joback Method
vc	2.058	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1883.32	J/molxK	1066.36	Joback Method
cpg	1916.97	J/molxK	1116.01	Joback Method
cpg	1948.24	J/molxK	1165.65	Joback Method
cpg	1977.48	J/molxK	1215.30	Joback Method
cpg	2004.99	J/molxK	1264.95	Joback Method
cpg	2031.10	J/molxK	1314.60	Joback Method
cpg	2056.13	J/molxK	1364.24	Joback Method
dvisc	0.0002681	Paxs	544.01	Joback Method
dvisc	0.0001000	Paxs	631.07	Joback Method

dvisc	0.0000473	Paxs	718.13	Joback Method
dvisc	0.0000264	Paxs	805.19	Joback Method
dvisc	0.0000164	Paxs	892.24	Joback Method
dvisc	0.0000112	Paxs	979.30	Joback Method
dvisc	0.0000081	Paxs	1066.36	Joback Method

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108514&amp;Units=SI</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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