

# Phenazepam

<b>Inchi:</b>	InChI=1S/C15H10BrClN2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)
<b>InchiKey:</b>	CGMJQQJSWIRRRLL-UHFFFAOYSA-N
<b>Formula:</b>	C15H10BrClN2O
<b>SMILES:</b>	O=C1CN=C(c2ccccc2Cl)c2cc(Br)ccc2N1
<b>Mol. weight [g/mol]:</b>	349.61
<b>CAS:</b>	66173-95-3

## Physical Properties

Property code	Value	Unit	Source
gf	420.23	kJ/mol	Joback Method
hf	194.52	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	85.08	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.892		Crippen Method
mvol	210.800	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	908.65	K	Joback Method
tc	1209.16	K	Joback Method
tf	712.14	K	Joback Method
vc	0.791	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.37	J/molxK	908.65	Joback Method
cpg	583.75	J/molxK	958.73	Joback Method
cpg	593.17	J/molxK	1008.82	Joback Method
cpg	600.64	J/molxK	1058.90	Joback Method
cpg	606.19	J/molxK	1108.99	Joback Method
cpg	609.84	J/molxK	1159.07	Joback Method
cpg	611.61	J/molxK	1209.16	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C66173953&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C66173953&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>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>hvpap:</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>rinppl:</b>	Non-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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