

# 2,5-Dichlorobenzylamine

<b>Inchi:</b>	InChI=1S/C7H7Cl2N/c8-6-1-2-7(9)5(3-6)4-10/h1-3H,4,10H2
<b>InchiKey:</b>	AKGJLIXNRPNPCH-UHFFFAOYSA-N
<b>Formula:</b>	C7H7Cl2N
<b>SMILES:</b>	NCc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	176.04
<b>CAS:</b>	10541-69-2

## Physical Properties

Property code	Value	Unit	Source
gf	143.80	kJ/mol	Joback Method
hf	28.09	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.452		Crippen Method
mcvol	120.190	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	543.59	K	Joback Method
tc	783.56	K	Joback Method
tf	363.21	K	Joback Method
vc	0.447	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.87	J/molxK	543.59	Joback Method
cpg	242.40	J/molxK	583.58	Joback Method
cpg	251.28	J/molxK	623.58	Joback Method
cpg	259.54	J/molxK	663.57	Joback Method
cpg	267.20	J/molxK	703.57	Joback Method
cpg	274.29	J/molxK	743.56	Joback Method
cpg	280.86	J/molxK	783.56	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=C10541692&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10541692&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>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>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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