

# 4-Acetamidobenzyl chloride

<b>Other names:</b>	Acetamide, N-[4-(chloromethyl)phenyl]- N-[4-Chloromethyl)phenyl]-acetamide
<b>Inchi:</b>	InChI=1S/C9H10ClNO/c10-6-8-3-1-7(2-4-8)5-9(11)12/h1-4H,5-6H2,(H2,11,12)
<b>InchiKey:</b>	DDKYWWMTJDDHKO-UHFFFAOYSA-N
<b>Formula:</b>	C9H10ClNO
<b>SMILES:</b>	NC(=O)Cc1ccc(CCl)cc1
<b>Mol. weight [g/mol]:</b>	183.63
<b>CAS:</b>	54777-65-0

## Physical Properties

Property code	Value	Unit	Source
gf	53.28	kJ/mol	Joback Method
hf	-98.56	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.453		Crippen Method
mvol	137.700	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	600.81	K	Joback Method
tc	834.00	K	Joback Method
tf	393.24	K	Joback Method
vc	0.515	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.94	J/molxK	600.81	Joback Method
cpg	322.44	J/molxK	639.67	Joback Method
cpg	333.12	J/molxK	678.54	Joback Method
cpg	343.04	J/molxK	717.40	Joback Method
cpg	352.21	J/molxK	756.27	Joback Method
cpg	360.69	J/molxK	795.13	Joback Method
cpg	368.51	J/molxK	834.00	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=C54777650&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54777650&amp;Units=SI</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>h vap:</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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