

# 2-(Alpha-methylphenethylamino)ethanethiol

<b>Inchi:</b>	InChI=1S/C11H17NS/c1-10(12-7-8-13)9-11-5-3-2-4-6-11/h2-6,10,12-13H,7-9H2,1H3
<b>InchiKey:</b>	GKRABYJWCXOEQF-UHFFFAOYSA-N
<b>Formula:</b>	C11H17NS
<b>SMILES:</b>	CC(Cc1ccccc1)NCCS
<b>Mol. weight [g/mol]:</b>	195.32
<b>CAS:</b>	20640-10-2

## Physical Properties

Property code	Value	Unit	Source
gf	270.49	kJ/mol	Joback Method
hf	52.83	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.137		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	590.35	K	Joback Method
tc	817.31	K	Joback Method
tf	314.27	K	Joback Method
vc	0.626	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.25	J/molxK	590.35	Joback Method
cpg	420.51	J/molxK	628.18	Joback Method
cpg	435.69	J/molxK	666.00	Joback Method
cpg	449.85	J/molxK	703.83	Joback Method
cpg	463.03	J/molxK	741.65	Joback Method
cpg	475.29	J/molxK	779.48	Joback Method
cpg	486.67	J/molxK	817.31	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20640102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20640102&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>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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