

Benzenemethanol, 2-(methylamino)-

Other names:	Benzyol alcohol, o-(methylamino)- o-(Methylamino)benzyol alcohol [2-(Methylamino)phenyl]methanol
Inchi:	InChI=1S/C8H11NO/c1-9-8-5-3-2-4-7(8)6-10/h2-5,9-10H,6H2,1H3
InchiKey:	ZWIBBLPQTVLYKW-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	CNc1ccccc1CO
Mol. weight [g/mol]:	137.18
CAS:	29055-08-1

Physical Properties

Property code	Value	Unit	Source
gf	71.83	kJ/mol	Joback Method
hf	-82.15	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.221		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
ripol	2476.00		NIST Webbook
tb	556.45	K	Joback Method
tc	756.18	K	Joback Method
tf	332.34	K	Joback Method
vc	0.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.75	J/molxK	556.45	Joback Method
cpg	277.34	J/molxK	589.74	Joback Method
cpg	287.33	J/molxK	623.03	Joback Method

cpg	296.74	J/mol×K	656.32	Joback Method
cpg	305.61	J/mol×K	689.61	Joback Method
cpg	313.95	J/mol×K	722.89	Joback Method
cpg	321.79	J/mol×K	756.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29055081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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