

Mebenzazine

Other names:	mebanazine
Inchi:	InChI=1S/C8H12N2/c1-7(10-9)8-5-3-2-4-6-8/h2-7,10H,9H2,1H3
InchiKey:	HHRZAEJMHSGZNP-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CC(NN)c1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	65-64-5

Physical Properties

Property code	Value	Unit	Source
gf	282.29	kJ/mol	Joback Method
hf	110.06	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.211		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1240.00		NIST Webbook
tb	531.38	K	Joback Method
tc	759.95	K	Joback Method
tf	327.26	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.51	J/molxK	531.38	Joback Method
cpg	287.05	J/molxK	569.48	Joback Method
cpg	299.68	J/molxK	607.57	Joback Method
cpg	311.44	J/molxK	645.67	Joback Method
cpg	322.37	J/molxK	683.76	Joback Method
cpg	332.52	J/molxK	721.86	Joback Method
cpg	341.93	J/molxK	759.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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