

Cyclooctanamine

Other names:	Cyclooctylamine Aminocyclooctane
Inchi:	InChI=1S/C8H17N/c9-8-6-4-2-1-3-5-7-8/h8H,1-7,9H2
InchiKey:	HSOHBWMXECKEKV-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	NC1CCCCCCC1
Mol. weight [g/mol]:	127.23
CAS:	5452-37-9

Physical Properties

Property code	Value	Unit	Source
gf	83.18	kJ/mol	Joback Method
hf	-132.66	kJ/mol	Joback Method
hfus	9.31	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.058		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	463.20	K	NIST Webbook
tc	715.19	K	Joback Method
tf	263.52	K	Joback Method
vc	0.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.51	J/mol×K	483.06	Joback Method
cpg	296.52	J/mol×K	521.75	Joback Method
cpg	315.43	J/mol×K	560.44	Joback Method
cpg	333.23	J/mol×K	599.12	Joback Method
cpg	349.94	J/mol×K	637.81	Joback Method
cpg	365.59	J/mol×K	676.50	Joback Method
cpg	380.18	J/mol×K	715.19	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5452379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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