

Cycloheptylamine

Other names:	Aminocycloheptane Cycloheptanamine- cycloheptanamine
Inchi:	InChI=1S/C7H15N/c8-7-5-3-1-2-4-6-7/h7H,1-6,8H2
InchiKey:	VXVVUHQULXCUPF-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	NC1CCCCC1
Mol. weight [g/mol]:	113.20
CAS:	5452-35-7

Physical Properties

Property code	Value	Unit	Source
gf	86.86	kJ/mol	Joback Method
hf	-105.86	kJ/mol	Joback Method
hfus	8.82	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.668		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	455.91	K	Joback Method
tc	682.69	K	Joback Method
tf	255.77	K	Joback Method
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.25	J/mol×K	455.91	Joback Method
cpg	250.11	J/mol×K	493.71	Joback Method
cpg	267.00	J/mol×K	531.50	Joback Method
cpg	282.93	J/mol×K	569.30	Joback Method
cpg	297.92	J/mol×K	607.10	Joback Method
cpg	312.00	J/mol×K	644.90	Joback Method

cpg

325.18

J/mol×K

682.69

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.20	K	1.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5452357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K.	https://www.doi.org/10.1016/j.jct.2011.04.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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