

2-(1-Cyclohexenyl)ethylamine

Other names:	1-Cyclohexene-1-ethanamine «beta»-(1-Cyclohexenyl)ethylamine Cyclohexenylethylamine 1-Cyclohexen-1-ylethylamine 2-(1-Cyclohexen-1-yl)ethylamine cyclohex-1-ene-1-ethylamine
Inchi:	InChI=1S/C8H15N/c9-7-6-8-4-2-1-3-5-8/h4H,1-3,5-7,9H2
InchiKey:	IUDMXOOVKMKODN-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	NCCC1=CCCCC1
Mol. weight [g/mol]:	125.21
CAS:	3399-73-3

Physical Properties

Property code	Value	Unit	Source
gf	135.42	kJ/mol	Joback Method
hf	-53.69	kJ/mol	Joback Method
hfus	13.27	kJ/mol	Joback Method
hvap	45.73	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.836		Crippen Method
mcvol	118.400	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	483.33	K	Joback Method
tc	701.79	K	Joback Method
tf	288.08	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.91	J/mol×K	483.33	Joback Method
cpg	276.58	J/mol×K	519.74	Joback Method
cpg	291.36	J/mol×K	556.15	Joback Method

cpg	305.28	J/mol×K	592.56	Joback Method
cpg	318.37	J/mol×K	628.97	Joback Method
cpg	330.66	J/mol×K	665.38	Joback Method
cpg	342.20	J/mol×K	701.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.70	K	0.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3399733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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