

(S)-(+)-1-Cyclohexylethylamine

Inchi:	InChI=1S/C8H17N/c1-7(9)8-5-3-2-4-6-8/h7-8H,2-6,9H2,1H3/t7-/m1/s1
InchiKey:	XBWOPGDJMAJJDG-SSDOTTSWSA-N
Formula:	C8H17N
SMILES:	CC(N)C1CCCCC1
Mol. weight [g/mol]:	127.23
CAS:	17430-98-7

Physical Properties

Property code	Value	Unit	Source
gf	104.94	kJ/mol	Joback Method
hf	-125.62	kJ/mol	Joback Method
hfus	9.98	kJ/mol	Joback Method
hvap	44.08	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.914		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	474.08	K	Joback Method
tc	693.89	K	Joback Method
tf	255.56	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.91	J/mol×K	474.08	Joback Method
cpg	295.18	J/mol×K	510.72	Joback Method
cpg	312.43	J/mol×K	547.35	Joback Method
cpg	328.69	J/mol×K	583.99	Joback Method
cpg	344.00	J/mol×K	620.62	Joback Method
cpg	358.38	J/mol×K	657.26	Joback Method
cpg	371.86	J/mol×K	693.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46083e+01
Coeff. B	-3.75135e+03
Coeff. C	-6.36950e+01
Temperature range (K), min.	325.65
Temperature range (K), max.	467.20

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17430987&Units=SI

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
pvap:	Vapor 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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