(1S,2S)-(+)-1,2-Diaminocyclohexane

Other names:	(+)-S,S-1,2-Diaminocyclohexane
	(-)-(1R,2R)-diaminocyclohexane
	(-)-trans-1,2-cyclohexanediamine
	(1R,2R)-1,2-cyclohexanediamine
	(1R,2R)-cyclohexane-1,2-diamine
	(R,R)-DACH
	1,2-Cyclohexanediamine, (1S,2S)-
	SS-Jacobsen Catalyst 2
Inchi:	InChI=1S/C6H14N2/c7-5-3-1-2-4-6(5)8/h5-6H,1-4,7-8H2/t5-,6-/m1/s1
InchiKey:	SSJXIUAHEKJCMH-PHDIDXHHSA-N
Formula:	C6H14N2
SMILES:	NC1CCCCC1N
Mol. weight [g/mol]:	114.19
CAS:	21436-03-3

Physical Properties

Property code	Value	Unit	Source
gf	149.28	kJ/mol	Joback Method
hf	-65.61	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.215		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	496.62	K	Joback Method
tc	730.03	K	Joback Method
tf	327.04	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.11	J/mol×K	496.62	Joback Method

cpg	266.28	J/mol×K	535.52	Joback Method
cpg	281.50	J/mol×K	574.42	Joback Method
cpg	295.80	J/mol×K	613.32	Joback Method
cpg	309.20	J/mol×K	652.22	Joback Method
cpg	321.72	J/mol×K	691.13	Joback Method
cpg	333.38	J/mol×K	730.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	5.30	NIST Webbook

Sources

Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for extraction of (1R,2R)-(-)-1,2-Diaminocyclohexane from aqueous solution with C4-C5 alcohols at different temperatures: https://www.doi.org/10.1016/j.jct.2018.01.013

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=C21436033&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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