Cyclohexanol, 2-amino-, cis-

Other names: cis-2-Aminocyclohexanol
2-Aminocyclohexanol, cis
Inchi: InChI=1S/C6H13NO/c7-5-3-1-2-4-6(5)8/h5-6,8H,1-4,7H2/t5-,6+/m1/s1
InchiKey: PQMCFTMVQORYJC-RITPCOANSA-N
Formula: C6H13NO
SMILES: NC1CCCCC1O
Mol. weight [g/mol]: 115.17
CAS: 931-15-7

Physical Properties

Property code	Value	Unit	Source
gf	-53.99	kJ/mol	Joback Method
hf	-251.63	kJ/mol	Joback Method
hfus	13.49	kJ/mol	Joback Method
hvap	56.39	kJ/mol	Joback Method
ie	9.59	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	0.249		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	516.27	K	Joback Method
tc	722.46	K	Joback Method
tf	380.50 ± 0.50	K	NIST Webbook
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.09	J/mol×K	516.27	Joback Method
cpg	259.48	J/mol×K	550.64	Joback Method
cpg	272.17	J/mol×K	585.00	Joback Method
cpg	284.16	J/mol×K	619.37	Joback Method
cpg	295.48	J/mol×K	653.73	Joback Method
cpg	306.14	J/mol×K	688.10	Joback Method

cpg	316.16	J/mol×K	722.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.00 ± 1.00	K	2.00	NIST Webbook

Sources

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=C931157&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
ie: Ionization energy
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