

trans-2-Aminocyclohexanol

Other names:	Cyclohexanol,2-amino-,trans- 2-Aminocyclohexanol, (E)-
Inchi:	InChI=1S/C6H13NO/c7-5-3-1-2-4-6(5)8/h5-6,8H,1-4,7H2/t5-,6-/m0/s1
InchiKey:	PQMCFTMVQORYJC-WDSKDSINSA-N
Formula:	C6H13NO
SMILES:	NC1CCCCC1O
Mol. weight [g/mol]:	115.17
CAS:	6982-39-4

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	9.49	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	341.00	K	NIST Webbook
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.09	J/molxK	516.27	Joback Method
cpg	259.48	J/molxK	550.64	Joback Method
cpg	272.17	J/molxK	585.00	Joback Method
cpg	284.16	J/molxK	619.37	Joback Method
cpg	295.48	J/molxK	653.73	Joback Method
cpg	306.14	J/molxK	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/ci9903071
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=C6982394&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

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