1-Hexanol, 6-amino-

Other names:	1-Amino-6-hexanol
	6-Amino-1-hexanol
	6-Aminohexanol
	6-Aminohexyl alcohol
	6-Hydroxyhexylamine
	6-aminohexan-1-ol
	Amidohexylalkohol
	Aminohexyl alcohol
	H2NCH2(CH2)4CH2OH
	Hexanol, 6-amino-
	NH2(CH2)6OH
	NSC 91538
Inchi:	InChI=1S/C6H15NO/c7-5-3-1-2-4-6-8/h8H,1-7H2
InchiKey:	SUTWPJHCRAITLU-UHFFFAOYSA-N
Formula:	C6H15NO
SMILES:	NCCCCCCO
Mol. weight [g/mol]:	117.19
CAS:	4048-33-3

Physical Properties

Property code	Value	Unit	Source
affp	969.00	kJ/mol	NIST Webbook
basg	915.70	kJ/mol	NIST Webbook
gf	-70.73	kJ/mol	Joback Method
hf	-285.61	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	56.27	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.498		Crippen Method
mcvol	111.250	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1156.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1902.00		NIST Webbook
tb	501.39	K	Joback Method

tc	674.34	K	Joback Method
tf	330.00 ± 1.00	K	NIST Webbook
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.58	J/mol×K	501.39	Joback Method
cpg	270.56	J/mol×K	530.21	Joback Method
cpg	280.12	J/mol×K	559.04	Joback Method
cpg	289.29	J/mol×K	587.86	Joback Method
cpg	298.06	J/mol×K	616.69	Joback Method
cpg	306.46	J/mol×K	645.51	Joback Method
cpg	314.50	J/mol×K	674.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.70	K	4.00	NIST Webbook
tbrp	410.50 ± 2.50	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76652e+01
Coeff. B	-5.35334e+03
Coeff. C	-8.18600e+01
Temperature range (K), min.	389.92
Temperature range (K), max.	515.20

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=C4048333&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume