2-Heptanol, 6-amino-2-methyl-

Other names: 2-Methyl-2-hydroxy-6-aminoheptane
6-Amino-2-methyl-2-heptanol
Heptaminol
Inchi: InChI=1S/C8H19NO/c1-7(9)5-4-6-8(2,3)10/h7,10H,4-6,9H2,1-3H3
InchiKey: LREQLEBVOXIEOM-UHFFFAOYSA-N
Formula: C8H19NO
SMILES: CC(N)CCCC(C)(C)O
Mol. weight [g/mol]: 145.24
CAS: 372-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-53.49	kJ/mol	Joback Method
hf	-340.92	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.275		Crippen Method
mcvol	139.430	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1118.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	543.48	K	Joback Method
tc	726.42	K	Joback Method
tf	311.42	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.36	J/mol×K	543.48	Joback Method

cpg	366.13	J/mol×K	573.97	Joback Method
cpg	378.24	J/mol×K	604.46	Joback Method
cpg	389.71	J/mol×K	634.95	Joback Method
cpg	400.58	J/mol×K	665.44	Joback Method
cpg	410.87	J/mol×K	695.93	Joback Method
cpg	420.62	J/mol×K	726.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.15423e+01
Coeff. B	-3.23212e+03
Coeff. C	-7.07400e+01
Temperature range (K), min.	357.92
Temperature range (K), max.	589.47

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C372667&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume