3-Pentanamine

Other names:	1-Ethylpropylamine
	3-Aminopentane
	3-Amylamine
	3-Pentylamine
	Propylamine, 1-ethyl-
	«alpha»-Ethylpropylamine
	Â«alphaÂ»-Ethylpropylamine
Inchi:	InChI=1S/C5H13N/c1-3-5(6)4-2/h5H,3-4,6H2,1-2H3
InchiKey:	PQPFFKCJENSZKL-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CCC(N)CC
Mol. weight [g/mol]:	87.16
CAS:	616-24-0

Physical Properties

Property code	Value	Unit	Source
gf	55.23	kJ/mol	Joback Method
hf	-118.02	kJ/mol	Joback Method
hfus	10.38	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.134		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	364.15 ± 2.00	K	NIST Webbook
tb	360.15 ± 3.00	K	NIST Webbook
tb	362.15 ± 3.00	K	NIST Webbook
tb	364.00	K	NIST Webbook
tb	364.20	K	NIST Webbook
tb	364.00 ± 3.00	K	NIST Webbook
tc	571.20	K	Joback Method
tf	214.37	K	Joback Method
vc	0.339	m3/kmol	Joback Method
volm	1.17e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.57	J/mol×K	385.89	Joback Method
cpg	184.03	J/mol×K	416.77	Joback Method
cpg	194.06	J/mol×K	447.66	Joback Method
cpg	203.68	J/mol×K	478.54	Joback Method
cpg	212.89	J/mol×K	509.43	Joback Method
cpg	221.72	J/mol×K	540.31	Joback Method
cpg	230.17	J/mol×K	571.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55255e+01
Coeff. B	-3.50307e+03
Coeff. C	-4.18280e+01
Temperature range (K), min.	271.72
Temperature range (K), max.	384.80

Sources

Benchmarks for the fifth industrial fluid properties simulation challenge:	https://www.doi.org/10.1016/j.fluid.2009.07.004
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
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=C616240&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume