Tuaminoheptane

Other names:	(.+/-.)-2-Aminoheptane
	1-Methylhexanamine
	1-Methylhexylamine
	2-Aminoheptane
	2-Heptanamine
	2-Heptylamine
	Armeen L-7
	DL-2-Aminoheptane
	Heptamine
	Heptamine, sympathomimetic
	Heptedrine
	Heptin
	Hexylamine, 1-methyl-
	NSC 1091
	Rineptil
	Rineptyl
	Tuamine
	Tuaminoheptan
Inchi:	InChI=1S/C7H17N/c1-3-4-5-6-7(2)8/h7H,3-6,8H2,1-2H3
InchiKey:	VSRBKQFNFZQRBM-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCCCC(C)N
Mol. weight [g/mol]:	115.22
CAS:	123-82-0

Physical Properties

Property code	Value	Unit	Source
gf	72.07	kJ/mol	Joback Method
hf	-159.30	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	41.43	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.914		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	810.00		NIST Webbook

rinpol	807.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	863.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1079.00		NIST Webbook
tb	415.20	K	NIST Webbook
tb	414.15 ± 3.00	K	NIST Webbook
tc	598.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	236.91	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.75	J/mol×K	431.65	Joback Method
cpg	263.71	J/mol×K	462.11	Joback Method
cpg	276.13	J/mol×K	492.56	Joback Method
cpg	288.03	J/mol×K	523.02	Joback Method
cpg	299.42	J/mol×K	553.48	Joback Method
cpg	310.31	J/mol×K	583.94	Joback Method
cpg	320.73	J/mol×K	614.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56533e+01
Coeff. B	-3.95757e+03
Coeff. C	-5.65620e+01
Temperature range (K), min.	314.12
Temperature range (K), max.	439.24

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
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=C123820&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

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