1-Heptanamine, N,N-diheptyl-

Other names: Triheptylamine
tri-n-Heptylamine
Inchi: InChI=1S/C21H45N/c1-4-7-10-13-16-19-22(20-17-14-11-8-5-2)21-18-15-12-9-6-3/h4-21H
InchiKey: CLZGJKHEVKJLLS-UHFFFAOYSA-N
Formula: C21H45N
SMILES: CCCCCCCN(CCCCCCC)CCCCCCC
Mol. weight [g/mol]: 311.59
CAS: 2411-36-1

Physical Properties

Property code	Value	Unit	Source
gf	236.72	kJ/mol	Joback Method
hf	-409.24	kJ/mol	Joback Method
hfus	53.17	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.200		Crippen Method
mcvol	316.730	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	603.15 ± 4.00	K	NIST Webbook
tc	854.82	K	Joback Method
tf	358.90	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.23	J/mol×K	692.32	Joback Method
cpg	965.83	J/mol×K	719.40	Joback Method
cpg	986.49	J/mol×K	746.49	Joback Method
cpg	1006.26	J/mol×K	773.57	Joback Method
cpg	1025.16	J/mol×K	800.65	Joback Method

cpg	1043.22	J/mol×K	827.74	Joback Method
cpg	1060.49	J/mol×K	854.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57300e+01
Coeff. B	-5.49279e+03
Coeff. C	-1.08826e+02
Temperature range (K), min.	464.52
Temperature range (K), max.	636.04

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2411361&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

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