1-Heptanamine, N-heptyl-

Other names: Di-n-heptylamine
Diheptylamine
N-heptyl-1-heptanamine
Inchi: InChI=1S/C14H31N/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h15H,3-14H2,1-2H3
InchiKey: NJWMENBYMFZACG-UHFFFAOYSA-N
Formula: C14H31N
SMILES: CCCCCCCNCCCCCCC
Mol. weight [g/mol]: 213.40
CAS: 2470-68-0

Physical Properties

Property code	Value	Unit	Source
gf	156.39	kJ/mol	Joback Method
hf	-278.82	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.517		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	545.65 ± 5.00	K	NIST Webbook
tb	544.15 ± 3.00	K	NIST Webbook
tb	548.15 ± 10.00	K	NIST Webbook
tc	732.88	K	Joback Method
tf	303.15 ± 2.00	K	NIST Webbook
tf	274.15 ± 1.00	K	NIST Webbook
tf	274.15 ± 1.00	K	NIST Webbook
tf	274.15 ± 2.00	K	NIST Webbook
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.82	J/mol×K	569.89	Joback Method
cpg	585.80	J/mol×K	597.06	Joback Method
cpg	603.06	J/mol×K	624.22	Joback Method
cpg	619.61	J/mol×K	651.39	Joback Method
cpg	635.48	J/mol×K	678.55	Joback Method
cpg	650.69	J/mol×K	705.72	Joback Method
cpg	665.26	J/mol×K	732.88	Joback Method
hvapt	81.20	kJ/mol	298.15	The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography
hvapt	60.00	kJ/mol	520.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57126e+01
Coeff. B	-5.01957e+03
Coeff. C	-9.27020e+01
Temperature range (K), min.	418.12
Temperature range (K), max.	575.30

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2470680&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

The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2013.08.005
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume