

4-N-Hexylaniline

Other names:	4-Hexylaniline Aniline, (p-hexyl)- Benzenamine, 4-hexyl- p-Hexylaniline p-n-Hexylaniline
Inchi:	InChI=1S/C12H19N/c1-2-3-4-5-6-11-7-9-12(13)10-8-11/h7-10H,2-6,13H2,1H3
InchiKey:	OVEMTTZEBOCJDV-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CCCCCc1ccc(N)cc1
Mol. weight [g/mol]:	177.29
CAS:	33228-45-4

Physical Properties

Property code	Value	Unit	Source
gf	219.39	kJ/mol	Joback Method
hf	-32.16	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.392		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	555.20	K	NIST Webbook
tc	787.94	K	Joback Method
tf	347.20	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.83	J/mol×K	578.15	Joback Method
cpg	426.97	J/mol×K	613.12	Joback Method
cpg	442.19	J/mol×K	648.08	Joback Method
cpg	456.54	J/mol×K	683.05	Joback Method

cpg	470.05	J/mol×K	718.01	Joback Method
cpg	482.75	J/mol×K	752.98	Joback Method
cpg	494.69	J/mol×K	787.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.50 ± 1.50	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50783e+01
Coeff. B	-4.66987e+03
Coeff. C	-9.12700e+01
Temperature range (K), min.	407.00
Temperature range (K), max.	569.41

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33228454&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/ci990307I
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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