N-Hexylaniline

Inchi: InChI=1S/C12H19N/c1-2-3-4-8-11-13-12-9-6-5-7-10-12/h5-7,9-10,13H,2-4,8,11H2,1H3
InchiKey: OXHJCNSXYDSOFN-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CCCCCCNc1ccccc1
Mol. weight [g/mol]: 177.29
CAS: 4746-32-1

Physical Properties

Property code	Value	Unit	Source
gf	251.96	kJ/mol	Joback Method
hf	-1.01	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
log10ws	-3.57		Crippen Method
logp	3.679		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	550.81	K	Joback Method
tc	751.21	K	Joback Method
tf	304.08	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.37	J/mol×K	550.81	Joback Method
cpg	415.02	J/mol×K	584.21	Joback Method
cpg	430.75	J/mol×K	617.61	Joback Method
cpg	445.59	J/mol×K	651.01	Joback Method
cpg	459.58	J/mol×K	684.41	Joback Method
cpg	472.75	J/mol×K	717.81	Joback Method
cpg	485.15	J/mol×K	751.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4746321&Units=SI
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume