Benzenamine, 4-(hexyloxy)-

Other names:	4-Hexyloxyaniline
	p-Hexyloxyaniline
	4-n-Hexyloxyaniline
	Aniline, (p-hexyloxy)-
Inchi:	InChI=1S/C12H19NO/c1-2-3-4-5-10-14-12-8-6-11(13)7-9-12/h6-9H,2-5,10,13H2,1H3
InchiKey:	DJRKHTCUXRGYEU-UHFFFAOYSA-N
Formula:	C12H19NO
SMILES:	CCCCCCOc1ccc(N)cc1
Mol. weight [g/mol]:	193.29
CAS:	39905-57-2

Physical Properties

Property code	Value	Unit	Source
gf	114.39	kJ/mol	Joback Method
hf	-164.38	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.228		Crippen Method
mcvol	172.030	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
tb	600.57	K	Joback Method
tc	808.14	K	Joback Method
tf	369.43	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.00	J/mol×K	600.57	Joback Method
cpg	452.77	J/mol×K	635.17	Joback Method
cpg	467.69	J/mol×K	669.76	Joback Method
cpg	481.77	J/mol×K	704.36	Joback Method
cpg	495.05	J/mol×K	738.95	Joback Method

cpg	507.54	J/mol×K	773.55	Joback Method
cpg	519.25	J/mol×K	808.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.70	K	0.70	NIST Webbook
tbrp	441.00 ± 1.00	K	0.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39905572&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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