4-Pentyloxyaniline

Other names: p-Pentyloxyaniline
Benzenamine, 4-(pentyloxy)-
Inchi: InChI=1S/C11H17NO/c1-2-3-4-9-13-11-7-5-10(12)6-8-11/h5-8H,2-4,9,12H2,1H3
InchiKey: QZLNSNIHXKQIIS-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: CCCCCOc1ccc(N)cc1
Mol. weight [g/mol]: 179.26
CAS: 39905-50-5

Physical Properties

Property code	Value	Unit	Source
gf	105.97	kJ/mol	Joback Method
hf	-143.74	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.838		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	577.69	K	Joback Method
tc	788.62	K	Joback Method
tf	358.16	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.97	J/mol×K	577.69	Joback Method
cpg	403.07	J/mol×K	612.85	Joback Method
cpg	417.36	J/mol×K	648.00	Joback Method
cpg	430.84	J/mol×K	683.16	Joback Method
cpg	443.55	J/mol×K	718.31	Joback Method
cpg	455.51	J/mol×K	753.47	Joback Method
cpg	466.72	J/mol×K	788.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.50 ± 0.50	K	2.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39905505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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