

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:	QZLNSNIH XKQIIS-UHFFFAOYSA-N
Formula:	C11H17NO
SMILES:	CCCCCOc1ccc(N)cc1
Mol. weight [g/mol]:	179.26

Physical Properties

Property code	Value	Unit	Source
hfus	24.28	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Cheméo Relay (1.0)
ie	7.37	eV	Cheméo Relay (1.0)
log10ws	-3.09		Cheméo Relay (1.0)
logp	2.838		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
tb	565.77	K	Cheméo Relay (1.0)
tf	308.67	K	Cheméo Relay (1.0)

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39905505&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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