Benzaldehyde, 4-pentyl-

Other names:	p-Pentylbenzaldehyde
	4-n-Amylbenzaldehyde
	4-pentylbenzaldehyde
Inchi:	InChI=1S/C12H16O/c1-2-3-4-5-11-6-8-12(10-13)9-7-11/h6-10H,2-5H2,1H3
InchiKey:	NQVZPRUSNWNSQH-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CCCCCc1ccc(C=O)cc1
Mol. weight [g/mol]:	176.25
CAS:	6853-57-2

Physical Properties

Property code	Value	Unit	Source
gf	53.42	kJ/mol	Joback Method
hf	-151.53	kJ/mol	Joback Method
hfus	22.78	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.232		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1463.00		NIST Webbook
ripol	2003.00		NIST Webbook
tb	554.28	K	Joback Method
tc	758.60	K	Joback Method
tf	305.94	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.99	J/mol×K	554.28	Joback Method
cpg	435.54	J/mol×K	724.54	Joback Method
cpg	423.76	J/mol×K	690.49	Joback Method
cpg	411.25	J/mol×K	656.44	Joback Method
cpg	397.97	J/mol×K	622.39	Joback Method
cpg	383.90	J/mol×K	588.33	Joback Method
cpg	446.62	J/mol×K	758.60	Joback Method
dvisc	0.0002416	Pa×s	554.28	Joback Method
dvisc	0.0003057	Pa×s	512.89	Joback Method
dvisc	0.0004030	Pa×s	471.50	Joback Method
dvisc	0.0005604	Pa×s	430.11	Joback Method
dvisc	0.0008359	Pa×s	388.72	Joback Method
dvisc	0.0013715	Pa×s	347.33	Joback Method
dvisc	0.0025728	Pa×s	305.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.00	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6853572&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
dvisc: Dynamic viscosity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume