

Benzaldehyde, 4-(hexyloxy)-

Other names:	4-Hexyloxybenzaldehyde p-Hexyloxybenzaldehyde 4-n-Hexyloxybenzaldehyde p-Hexoxybenzaldehyde p-n-Hexyloxybenzaldehyde Benzaldehyde, p-(hexyloxy)- 4-Hexoxybenzaldehyde
Inchi:	InChI=1S/C13H18O2/c1-2-3-4-5-10-15-13-8-6-12(11-14)7-9-13/h6-9,11H,2-5,10H2,1H3
InchiKey:	GWXUVWKBVROFDM-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCCCOc1ccc(C=O)cc1
Mol. weight [g/mol]:	206.28
CAS:	5736-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-43.16	kJ/mol	Joback Method
hf	-304.39	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.458		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
tb	599.58	K	Joback Method
tc	799.07	K	Joback Method
tf	339.44	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.39	J/molxK	599.58	Joback Method
cpg	511.75	J/molxK	765.82	Joback Method

cpg	499.61	J/molxK	732.57	Joback Method
cpg	486.73	J/molxK	699.33	Joback Method
cpg	473.07	J/molxK	666.08	Joback Method
cpg	458.64	J/molxK	632.83	Joback Method
cpg	523.16	J/molxK	799.07	Joback Method
dvisc	0.0001813	Paxs	599.58	Joback Method
dvisc	0.0002301	Paxs	556.22	Joback Method
dvisc	0.0003039	Paxs	512.87	Joback Method
dvisc	0.0004226	Paxs	469.51	Joback Method
dvisc	0.0006285	Paxs	426.15	Joback Method
dvisc	0.0010225	Paxs	382.80	Joback Method
dvisc	0.0018840	Paxs	339.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.00 ± 1.00	K	0.07	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=C5736947&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
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
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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