2-(Hexyloxy)benzaldehyde

Other names:	o-Hexyloxybenzaldehyde
	2-n-Hexyloxybenzaldehyde
	Benzaldehyde, 2-(hexyloxy)-
	Benzaldehyde, o-(n-hexyloxy)-,
Inchi:	InChI=1S/C13H18O2/c1-2-3-4-7-10-15-13-9-6-5-8-12(13)11-14/h5-6,8-9,11H,2-4,7,10H2
InchiKey:	IFOIDROUJIGQAV-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCCCOc1ccccc1C=O
Mol. weight [g/mol]:	206.28
CAS:	7162-59-6

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/mol×K	599.58	Joback Method
cpg	458.64	J/mol×K	632.83	Joback Method
cpg	473.07	J/mol×K	666.08	Joback Method
cpg	486.73	J/mol×K	699.33	Joback Method
cpg	499.61	J/mol×K	732.57	Joback Method

cpg	511.75	J/mol×K	765.82	Joback Method
cpg	523.16	J/mol×K	799.07	Joback Method
dvisc	0.0018840	Pa×s	339.44	Joback Method
dvisc	0.0010225	Pa×s	382.80	Joback Method
dvisc	0.0006285	Pa×s	426.15	Joback Method
dvisc	0.0004226	Pa×s	469.51	Joback Method
dvisc	0.0003039	Pa×s	512.87	Joback Method
dvisc	0.0002301	Pa×s	556.22	Joback Method
dvisc	0.0001813	Pa×s	599.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.50 ± 2.50	K	0.07	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7162596&Units=SI

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