Benzaldehyde, 2-hydroxy, 5-hexyl

Inchi: InChI=1S/C13H18O2/c1-2-3-4-5-6-11-7-8-13(15)12(9-11)10-14/h7-10,15H,2-6H2,1H3
InchiKey: AKLLVPQDWXRGLG-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCCCCc1ccc(O)c(C=O)c1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-92.78	kJ/mol	Joback Method
hf	-349.48	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	67.20	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.328		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1884.00		NIST Webbook
tb	657.78	K	Joback Method
tc	868.90	K	Joback Method
tf	428.93	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.92	J/mol×K	657.78	Joback Method
cpg	535.00	J/mol×K	833.71	Joback Method
cpg	523.91	J/mol×K	798.53	Joback Method
cpg	512.22	J/mol×K	763.34	Joback Method
cpg	499.88	J/mol×K	728.15	Joback Method
cpg	486.80	J/mol×K	692.97	Joback Method
cpg	545.58	J/mol×K	868.90	Joback Method
dvisc	0.0000258	Pa×s	657.78	Joback Method
dvisc	0.0000383	Pa×s	619.64	Joback Method

dvisc	0.0000599	Pa×s	581.50	Joback Method
dvisc	0.0000997	Pa×s	543.36	Joback Method
dvisc	0.0001793	Pa×s	505.21	Joback Method
dvisc	0.0003547	Pa×s	467.07	Joback Method
dvisc	0.0007924	Pa×s	428.93	Joback Method

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=R256883&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume