4-Hydroxyoctanophenone

Other names: 4'-Hydroxyoctanophenone
4-Octanoylphenol
Octanophenone, 4'-hydroxy-
Inchi: InChI=1S/C14H20O2/c1-2-3-4-5-6-7-14(16)12-8-10-13(15)11-9-12/h8-11,15H,2-7H2,1H3
InchiKey: GPDYSJOGSNWMDZ-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCCCC(=O)c1ccc(O)cc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
af	0.8101		Cheméo Relay (1.0)
hf	-398.01	kJ/mol	Cheméo Relay (1.0)
hfus	33.44	kJ/mol	Joback Method
hvap	93.92	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-4.25		Cheméo Relay (1.0)
logp	3.935		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	600.93	K	Cheméo Relay (1.0)
tc	813.85	K	Cheméo Relay (1.0)
tf	364.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.93	J/mol×K	680.89	Joback Method
cpg	539.78	J/mol×K	716.11	Joback Method
cpg	553.76	J/mol×K	751.32	Joback Method
cpg	566.94	J/mol×K	786.54	Joback Method
cpg	579.42	J/mol×K	821.76	Joback Method
cpg	591.26	J/mol×K	856.97	Joback Method
cpg	602.55	J/mol×K	892.19	Joback Method

dvisc	0.0007327	Pa×s	435.61	Joback Method
dvisc	0.0003067	Pa×s	476.49	Joback Method
dvisc	0.0001474	Pa×s	517.37	Joback Method
dvisc	0.0000788	Pa×s	558.25	Joback Method
dvisc	0.0000459	Pa×s	599.13	Joback Method
dvisc	0.0000287	Pa×s	640.01	Joback Method
dvisc	0.0000189	Pa×s	680.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2589733&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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