4'-HEXYLACETOPHENONE

Other names: 4-n-Hexylacetophenone
4'-n-Hexylacetophenone
Ethanone, 1-(4-hexylphenyl)-
Inchi: InChI=1S/C14H20O/c1-3-4-5-6-7-13-8-10-14(11-9-13)12(2)15/h8-11H,3-7H2,1-2H3
InchiKey: WWBVHJKFJZBRSO-UHFFFAOYSA-N
Formula: C14H20O
SMILES: CCCCCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
af	0.6454		Cheméo Relay (1.0)
gf	40.86	kJ/mol	Joback Method
hf	-236.40	kJ/mol	Cheméo Relay (1.0)
hfus	27.27	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-4.84		Cheméo Relay (1.0)
logp	4.012		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
tb	573.93	K	Cheméo Relay (1.0)
tc	772.20	K	Cheméo Relay (1.0)
tf	278.42	K	Cheméo Relay (1.0)
vc	0.700	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.80	J/mol×K	605.25	Joback Method
cpg	552.68	J/mol×K	808.08	Joback Method
cpg	540.43	J/mol×K	774.27	Joback Method
cpg	527.41	J/mol×K	740.47	Joback Method
cpg	513.56	J/mol×K	706.66	Joback Method

cpg	498.87	J/mol×K	672.86	Joback Method
cpg	483.29	J/mol×K	639.05	Joback Method
dvisc	0.0004505	Pa×s	470.83	Joback Method
dvisc	0.0001876	Pa×s	605.25	Joback Method
dvisc	0.0002398	Pa×s	560.44	Joback Method
dvisc	0.0003198	Pa×s	515.64	Joback Method
dvisc	0.0021783	Pa×s	336.41	Joback Method
dvisc	0.0006821	Pa×s	426.02	Joback Method
dvisc	0.0011385	Pa×s	381.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.50 ± 2.50	K	0.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=C37592726&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume