

p-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
CAS:	37592-72-6

Physical Properties

Property code	Value	Unit	Source
gf	40.86	kJ/mol	Joback Method
hf	-219.81	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.012		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
tb	605.25	K	Joback Method
tc	808.08	K	Joback Method
tf	336.41	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.80	J/molxK	605.25	Joback Method
cpg	540.43	J/molxK	774.27	Joback Method
cpg	527.41	J/molxK	740.47	Joback Method
cpg	513.56	J/molxK	706.66	Joback Method
cpg	498.87	J/molxK	672.86	Joback Method
cpg	483.29	J/molxK	639.05	Joback Method

cpg	552.68	J/mol×K	808.08	Joback Method
dvisc	0.0001876	Paxs	605.25	Joback Method
dvisc	0.0002398	Paxs	560.44	Joback Method
dvisc	0.0003198	Paxs	515.64	Joback Method
dvisc	0.0004505	Paxs	470.83	Joback Method
dvisc	0.0006821	Paxs	426.02	Joback Method
dvisc	0.0011385	Paxs	381.22	Joback Method
dvisc	0.0021783	Paxs	336.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C37592726&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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