p-Heptylacetophenone

Other names:	4-n-Heptylacetophenone
	4'-n-Heptylacetophenone
	Ethanone, 1-(4-heptylphenyl)-
	p-n-Heptylacetophenone
	4'-Heptylacetophenone
	1-(4-heptylphenyl)ethan-1-one
Inchi:	InChI=1S/C15H22O/c1-3-4-5-6-7-8-14-9-11-15(12-10-14)13(2)16/h9-12H,3-8H2,1-2H3
InchiKey:	UQBRZOXCKKBKDU-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CCCCCCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	218.33
CAS:	37593-03-6

Physical Properties

Property code	Value	Unit	Source
gf	49.28	kJ/mol	Joback Method
hf	-240.45	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.402		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
tb	628.13	K	Joback Method
tc	828.14	K	Joback Method
tf	347.68	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.31	J/mol×K	628.13	Joback Method
cpg	535.29	J/mol×K	661.46	Joback Method
cpg	551.33	J/mol×K	694.80	Joback Method

cpg	566.47	J/mol×K	728.13	Joback Method
cpg	580.73	J/mol×K	761.47	Joback Method
cpg	594.17	J/mol×K	794.80	Joback Method
cpg	606.81	J/mol×K	828.14	Joback Method
dvisc	0.0020914	Pa×s	347.68	Joback Method
dvisc	0.0010755	Pa×s	394.42	Joback Method
dvisc	0.0006368	Pa×s	441.16	Joback Method
dvisc	0.0004168	Pa×s	487.90	Joback Method
dvisc	0.0002938	Pa×s	534.65	Joback Method
dvisc	0.0002191	Pa×s	581.39	Joback Method
dvisc	0.0001707	Pa×s	628.13	Joback Method

Sources

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=C37593036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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