

Hexadecanophenone

Other names:	Pentadecyl phenyl ketone n-Hexadecanophenone 1-Hexadecanone, 1-phenyl-
Inchi:	InChI=1S/C22H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-22(23)21-18-15-14-16-19-21/
InchiKey:	IIOLAWJMOGLOIB-UHFFFAOYSA-N
Formula:	C22H36O
SMILES:	CCCCCCCCCCCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	316.52
CAS:	6697-12-7

Physical Properties

Property code	Value	Unit	Source
gf	117.85	kJ/mol	Joback Method
hf	-373.46	kJ/mol	Joback Method
hfus	48.38	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.351		Crippen Method
mcvol	298.650	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
tb	783.31	K	Joback Method
tc	973.54	K	Joback Method
tf	324.00 ± 3.00	K	NIST Webbook
tf	332.20 ± 0.60	K	NIST Webbook
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.68	J/mol×K	783.31	Joback Method
cpg	999.21	J/mol×K	941.84	Joback Method
cpg	984.04	J/mol×K	910.13	Joback Method
cpg	967.96	J/mol×K	878.43	Joback Method
cpg	950.90	J/mol×K	846.72	Joback Method

cpg	932.83	J/mol×K	815.02	Joback Method
cpg	1013.52	J/mol×K	973.54	Joback Method
dvisc	0.0000749	Pa×s	783.31	Joback Method
dvisc	0.0001000	Pa×s	721.77	Joback Method
dvisc	0.0001411	Pa×s	660.22	Joback Method
dvisc	0.0002135	Pa×s	598.68	Joback Method
dvisc	0.0003553	Pa×s	537.14	Joback Method
dvisc	0.0006747	Pa×s	475.59	Joback Method
dvisc	0.0015501	Pa×s	414.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	521.20	K	1.60	NIST Webbook

Sources

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=C6697127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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