TETRADECANOPHENONE

Other names:	Myristophenone
	1-Tetradecanone, 1-phenyl-
	Ketone, phenyl tridecyl
	Tridecyl phenyl ketone
Inchi:	InChI=1S/C20H32O/c1-2-3-4-5-6-7-8-9-10-11-15-18-20(21)19-16-13-12-14-17-19/h12-14
InchiKey:	LXUIUVLDNRQBQJ-UHFFFAOYSA-N
Formula:	C20H32O
SMILES:	CCCCCCCCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	288.47

Physical Properties

Property code	Value	Unit	Source
af	0.8731		Cheméo Relay (1.0)
gf	101.01	kJ/mol	Joback Method
hf	-345.11	kJ/mol	Cheméo Relay (1.0)
hfus	43.20	kJ/mol	Joback Method
hvap	103.58	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-6.83		Cheméo Relay (1.0)
logp	6.570		Crippen Method
mcvol	270.470	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
tb	617.14	K	Cheméo Relay (1.0)
tc	824.28	K	Cheméo Relay (1.0)
tf	321.82	K	Cheméo Relay (1.0)
vc	1.035	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.38	J/mol×K	737.55	Joback Method
cpg	814.06	J/mol×K	769.28	Joback Method
cpg	831.71	J/mol×K	801.02	Joback Method
cpg	848.37	J/mol×K	832.75	Joback Method

cpg	864.08	J/mol×K	864.49	Joback Method
cpg	878.89	J/mol×K	896.22	Joback Method
cpg	892.86	J/mol×K	927.95	Joback Method
dvisc	0.0018824	Pa×s	391.51	Joback Method
dvisc	0.0008365	Pa×s	449.18	Joback Method
dvisc	0.0004471	Pa×s	506.86	Joback Method
dvisc	0.0002716	Pa×s	564.53	Joback Method
dvisc	0.0001809	Pa×s	622.20	Joback Method
dvisc	0.0001291	Pa×s	679.88	Joback Method
dvisc	0.0000972	Pa×s	737.55	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C4497056&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume