DODECANOPHENONE

Other names: 1-Dodecanone, 1-phenyl-
1-Phenyl-1-dodecanone
1-phenyldodecan-1-one
Laurophenone
Phenyl n-undecyl ketone
Phenyl undecyl ketone
Undecyl phenyl ketone
n-Dodecanophenone

Inchi: InChI=1S/C18H28O/c1-2-3-4-5-6-7-8-9-13-16-18(19)17-14-11-10-12-15-17/h10-12,14-15

InchiKey: DJNJZIFFCJTUDS-UHFFFAOYSA-N

Formula: C18H28O

SMILES: CCCCCCCCCCCC(=O)c1ccccc1

Mol. weight [g/mol]: 260.42

Physical Properties

Property code	Value	Unit	Source
af	0.7994		Cheméo Relay (1.0)
gf	84.17	kJ/mol	Joback Method
hf	-302.30	kJ/mol	Cheméo Relay (1.0)
hfus	38.02	kJ/mol	Joback Method
hvap	94.60	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-6.21		Cheméo Relay (1.0)
logp	5.790		Crippen Method
mcvol	242.290	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
tb	603.25	K	Cheméo Relay (1.0)
tc	807.66	K	Cheméo Relay (1.0)
tf	314.44	K	Cheméo Relay (1.0)
vc	0.924	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	681.08	J/mol×K	691.79	Joback Method
cpg	775.91	J/mol×K	884.45	Joback Method
cpg	762.35	J/mol×K	852.34	Joback Method
cpg	747.95	J/mol×K	820.23	Joback Method
cpg	732.66	J/mol×K	788.12	Joback Method
cpg	716.45	J/mol×K	756.01	Joback Method
cpg	699.27	J/mol×K	723.90	Joback Method
dvisc	0.0003393	Pa×s	530.38	Joback Method
dvisc	0.0001242	Pa×s	691.79	Joback Method
dvisc	0.0001641	Pa×s	637.99	Joback Method
dvisc	0.0002282	Pa×s	584.18	Joback Method
dvisc	0.0022340	Pa×s	368.97	Joback Method
dvisc	0.0005518	Pa×s	476.58	Joback Method
dvisc	0.0010158	Pa×s	422.77	Joback Method

Sources

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=C1674380&Units=SI
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

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