

n-Undecanophenone

Other names:	1-Undecanone, 1-phenyl- 1-phenylundecanone
Inchi:	InChI=1S/C17H26O/c1-2-3-4-5-6-7-8-12-15-17(18)16-13-10-9-11-14-16/h9-11,13-14H,2-
InchiKey:	LHJBFOGCFZHBAJ-UHFFFAOYSA-N
Formula:	C17H26O
SMILES:	CCCCCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	246.39
CAS:	4433-30-1

Physical Properties

Property code	Value	Unit	Source
gf	75.75	kJ/mol	Joback Method
hf	-270.26	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.400		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	668.91	K	Joback Method
tc	863.35	K	Joback Method
tf	357.70	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.61	J/mol×K	668.91	Joback Method
cpg	643.52	J/mol×K	701.32	Joback Method
cpg	660.42	J/mol×K	733.72	Joback Method
cpg	676.37	J/mol×K	766.13	Joback Method
cpg	691.40	J/mol×K	798.54	Joback Method

cpg	705.55	J/mol×K	830.95	Joback Method
cpg	718.88	J/mol×K	863.35	Joback Method
dvisc	0.0024092	Pa×s	357.70	Joback Method
dvisc	0.0011092	Pa×s	409.57	Joback Method
dvisc	0.0006080	Pa×s	461.44	Joback Method
dvisc	0.0003763	Pa×s	513.31	Joback Method
dvisc	0.0002544	Pa×s	565.17	Joback Method
dvisc	0.0001836	Pa×s	617.04	Joback Method
dvisc	0.0001394	Pa×s	668.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4433301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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