1-UNDECANONE, 1-PHENYL-

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

Physical Properties

Property code	Value	Unit	Source
af	0.7612		Cheméo Relay (1.0)
gf	75.75	kJ/mol	Joback Method
hf	-280.68	kJ/mol	Cheméo Relay (1.0)
hfus	35.43	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-5.91		Cheméo Relay (1.0)
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	595.68	K	Cheméo Relay (1.0)
tc	798.50	K	Cheméo Relay (1.0)
tf	310.24	K	Cheméo Relay (1.0)
vc	0.868	m3/kmol	Cheméo Relay (1.0)

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	513.30	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

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=C4433301&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume