

n-Octyl phenyl ketone

Other names:

n-Nonanophenone
1-Nonanone, 1-phenyl-
1-Phenyl-1-nonanone
1-Phenylnonan-1-one

Inchi:

InChI=1S/C15H22O/c1-2-3-4-5-6-10-13-15(16)14-11-8-7-9-12-14/h7-9,11-12H,2-6,10,13

InchiKey:

PFUPABFCHVRLLY-UHFFFAOYSA-N

Formula:

C15H22O

SMILES:

CCCCCCCC(=O)c1ccccc1

Mol. weight [g/mol]:

218.33

CAS:

6008-36-2

Physical Properties

Property code	Value	Unit	Source
gf	58.91	kJ/mol	Joback Method
hf	-228.98	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.620		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	623.15	K	Joback Method
tc	822.26	K	Joback Method
tf	335.16	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.45	J/mol×K	623.15	Joback Method
cpg	535.64	J/mol×K	656.33	Joback Method
cpg	551.85	J/mol×K	689.52	Joback Method

cpg	567.13	J/molxK	722.70	Joback Method
cpg	581.52	J/molxK	755.89	Joback Method
cpg	595.04	J/molxK	789.07	Joback Method
cpg	607.76	J/molxK	822.26	Joback Method
dvisc	0.0027358	Paxs	335.16	Joback Method
dvisc	0.0012943	Paxs	383.16	Joback Method
dvisc	0.0007234	Paxs	431.16	Joback Method
dvisc	0.0004543	Paxs	479.15	Joback Method
dvisc	0.0003105	Paxs	527.15	Joback Method
dvisc	0.0002261	Paxs	575.15	Joback Method
dvisc	0.0001729	Paxs	623.15	Joback Method

Sources

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=C6008362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/20-198-0/n-Octyl-phenyl-ketone.pdf>

Generated by Cheméo on 2024-04-23 08:04:10.674494247 +0000 UTC m=+16148699.595071562.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.