10-Nonadecanone

Other names: Di-n-nonyl ketone
Dinonyl ketone
nonadecan-10-one
Inchi: InChI=1S/C19H38O/c1-3-5-7-9-11-13-15-17-19(20)18-16-14-12-10-8-6-4-2/h3-18H2,1-2
InchiKey: YUPOCHDBBHTUBJ-UHFFFAOYSA-N
Formula: C19H38O
SMILES: CCCCCCCCCC(=O)CCCCCCCCC
Mol. weight [g/mol]: 282.50
CAS: 504-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-19.82	kJ/mol	Joback Method
hf	-548.07	kJ/mol	Joback Method
hfus	46.56	kJ/mol	Joback Method
hvap	64.63	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.837		Crippen Method
mcvol	280.140	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	687.99	K	Joback Method
tc	855.89	K	Joback Method
tf	330.00 ± 0.10	K	NIST Webbook
tf	329.15 ± 1.50	K	NIST Webbook
tf	330.00 ± 0.50	K	NIST Webbook
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.83	J/mol×K	827.90	Joback Method

cpg	920.22	J/mol×K	855.89	Joback Method
cpg	816.10	J/mol×K	687.99	Joback Method
cpg	835.51	J/mol×K	715.97	Joback Method
cpg	854.06	J/mol×K	743.96	Joback Method
cpg	871.78	J/mol×K	771.94	Joback Method
cpg	888.70	J/mol×K	799.92	Joback Method
dvisc	0.0001094	Pa×s	687.99	Joback Method
dvisc	0.0001477	Pa×s	632.30	Joback Method
dvisc	0.0027375	Pa×s	353.82	Joback Method
dvisc	0.0011112	Pa×s	409.51	Joback Method
dvisc	0.0005597	Pa×s	465.21	Joback Method
dvisc	0.0003265	Pa×s	520.90	Joback Method
dvisc	0.0002113	Pa×s	576.60	Joback Method
hfust	66.67	kJ/mol	330.00	NIST Webbook
hfust	66.67	kJ/mol	330.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45877e+01
Coeff. B	-5.10168e+03
Coeff. C	-1.11522e+02
Temperature range (K), min.	468.28
Temperature range (K), max.	661.49

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C504574&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume