2-Nonadecanone

Other names:	Methyl heptadecyl ketone
	nonadecan-2-one
Inchi:	InChI=1S/C19H38O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)20/h3-18H2,1-2
InchiKey:	IEDKVDCIEARIIU-UHFFFAOYSA-N
Formula:	C19H38O
SMILES:	CCCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	282.50
CAS:	629-66-3

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	2100.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2090.70		NIST Webbook
rinpol	348.32		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	687.99	K	Joback Method
tc	855.89	K	Joback Method
tf	353.82	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.10	J/mol×K	687.99	Joback Method

cpg	904.83	J/mol×K	827.90	Joback Method
cpg	888.70	J/mol×K	799.92	Joback Method
cpg	871.78	J/mol×K	771.94	Joback Method
cpg	854.06	J/mol×K	743.96	Joback Method
cpg	835.51	J/mol×K	715.97	Joback Method
cpg	920.22	J/mol×K	855.89	Joback Method
dvisc	0.0001094	Pa×s	687.99	Joback Method
dvisc	0.0001477	Pa×s	632.30	Joback Method
dvisc	0.0002113	Pa×s	576.60	Joback Method
dvisc	0.0003265	Pa×s	520.90	Joback Method
dvisc	0.0005597	Pa×s	465.21	Joback Method
dvisc	0.0011112	Pa×s	409.51	Joback Method
dvisc	0.0027375	Pa×s	353.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47620e+01
Coeff. B	-5.18154e+03
Coeff. C	-1.12440e+02
Temperature range (K), min.	470.42
Temperature range (K), max.	660.72

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629663&Units=SI
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

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
pvap:	Vapor 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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