7-Tridecanone

Other names:	Dihexyl ketone
	Enanthone
	Hexyl ketone
	di-Normal-hexyl ketone
	di-n-Hexyl ketone
	tridecan-7-one
Inchi:	InChI=1S/C13H26O/c1-3-5-7-9-11-13(14)12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	ULIAPOFMBCCSPE-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	CCCCCCC(=O)CCCCCC
Mol. weight [g/mol]:	198.34
CAS:	462-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-70.34	kJ/mol	Joback Method
hf	-424.23	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rhoc	238.01 ± 7.93	kg/m3	NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	550.71	K	Joback Method
tc	708.20 ± 2.80	K	NIST Webbook
tf	286.20	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.38	J/mol×K	691.58	Joback Method
cpg	533.84	J/mol×K	635.23	Joback Method
cpg	518.60	J/mol×K	607.06	Joback Method
cpg	502.70	J/mol×K	578.88	Joback Method
cpg	486.12	J/mol×K	550.71	Joback Method
cpg	548.43	J/mol×K	663.40	Joback Method
cpg	575.73	J/mol×K	719.75	Joback Method
dvisc	0.0042194	Pa×s	286.20	Joback Method
dvisc	0.0002125	Pa×s	550.71	Joback Method
dvisc	0.0002816	Pa×s	506.62	Joback Method
dvisc	0.0003936	Pa×s	462.54	Joback Method
dvisc	0.0005905	Pa×s	418.46	Joback Method
dvisc	0.0009747	Pa×s	374.37	Joback Method
dvisc	0.0018390	Pa×s	330.28	Joback Method
hsubt	103.80	kJ/mol	290.00	NIST Webbook
hvapt	49.30	kJ/mol	509.50	NIST Webbook
hvapt	62.70	kJ/mol	497.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51968e+01
Coeff. B	-4.69904e+03
Coeff. C	-8.96440e+01
Temperature range (K), min.	404.82
Temperature range (K), max.	565.00

Sources

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=C462180&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume