18-Pentatriacontanone

Other names:	Di-n-heptadecyl ketone
	Di-stearyl ketone
	Diheptadecyl ketone
	Heptadecyl ketone
	Stearone
	Stearyl ketone
	pentatriacontan-18-one
Inchi:	InChI=1S/C35H70O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35(36)34-32-30-2
InchiKey:	DMCJFWXGXUEHFD-UHFFFAOYSA-N
Formula:	C35H70O
SMILES:	CCCCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	506.93
CAS:	504-53-0

Physical Properties

Property code	Value	Unit	Source
gf	114.90	kJ/mol	Joback Method
hf	-878.31	kJ/mol	Joback Method
hfus	88.00	kJ/mol	Joback Method
hvap	100.25	kJ/mol	Joback Method
log10ws	-13.75		Crippen Method
logp	13.079		Crippen Method
mcvol	505.580	ml/mol	McGowan Method
pc	490.55	kPa	Joback Method
tb	1054.07	K	Joback Method
tc	1349.17	K	Joback Method
tf	362.00 ± 1.00	K	NIST Webbook
tf	362.00 ± 1.50	K	NIST Webbook
vc	2.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1853.58	J/mol×K	1054.07	Joback Method

cpg	1886.45	J/mol×K	1103.25	Joback Method
cpg	1916.66	J/mol×K	1152.44	Joback Method
cpg	1944.50	J/mol×K	1201.62	Joback Method
cpg	1970.24	J/mol×K	1250.80	Joback Method
cpg	1994.17	J/mol×K	1299.99	Joback Method
cpg	2016.56	J/mol×K	1349.17	Joback Method
dvisc	0.0003643	Pa×s	534.14	Joback Method
dvisc	0.0001331	Pa×s	620.79	Joback Method
dvisc	0.0000622	Pa×s	707.45	Joback Method
dvisc	0.0000344	Pa×s	794.11	Joback Method
dvisc	0.0000213	Pa×s	880.76	Joback Method
dvisc	0.0000144	Pa×s	967.41	Joback Method
dvisc	0.0000104	Pa×s	1054.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.10683e+01
Coeff. B	-1.00908e+04
Coeff. C	-1.80133e+02
Temperature range (K), min.	665.72
Temperature range (K), max.	820.54

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=C504530&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume