16-HENTRIACONTANONE

Other names:	16-Hentricontanone
	Dipentadecyl ketone
	Hentricontan-16-one
	NSC 953
	Palmitone
	Pentadecyl ketone
Inchi:	InChI=1S/C31H62O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31(32)30-28-26-24-22-2
InchiKey:	UNRFDARCMOHDBJ-UHFFFAOYSA-N
Formula:	C31H62O
SMILES:	CCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	450.84
CAS:	502-73-8

Physical Properties

Property code	Value	Unit	Source
af	1.2937		Cheméo Relay (1.0)
gf	81.22	kJ/mol	Joback Method
hf	-814.76	kJ/mol	Cheméo Relay (1.0)
hfus	77.65	kJ/mol	Joback Method
hvap	148.13	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-10.30		Cheméo Relay (1.0)
logp	11.518		Crippen Method
mcvol	449.220	ml/mol	McGowan Method
pc	585.99	kPa	Joback Method
rinpol	3304.20		NIST Webbook
rinpol	3304.20		NIST Webbook
tb	658.08	K	Cheméo Relay (1.0)
tc	848.15	K	Cheméo Relay (1.0)
tf	356.40 ± 0.50	K	NIST Webbook
vc	1.761	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1701.41	J/mol×K	1158.02	Joback Method
cpg	1720.95	J/mol×K	1197.11	Joback Method
cpg	1608.78	J/mol×K	1001.64	Joback Method
cpg	1634.36	J/mol×K	1040.74	Joback Method
cpg	1658.24	J/mol×K	1079.83	Joback Method
cpg	1680.55	J/mol×K	1118.92	Joback Method
cpg	1581.38	J/mol×K	962.55	Joback Method
dvisc	0.0001141	Pa×s	646.89	Joback Method
dvisc	0.0002408	Pa×s	567.98	Joback Method
dvisc	0.0006463	Pa×s	489.06	Joback Method
dvisc	0.0000636	Pa×s	725.80	Joback Method
dvisc	0.0000398	Pa×s	804.72	Joback Method
dvisc	0.0000271	Pa×s	883.63	Joback Method
dvisc	0.0000196	Pa×s	962.55	Joback Method
hfust	117.10	kJ/mol	356.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.91463e+01
Coeff. B	-8.60629e+03
Coeff. C	-1.64565e+02
Temperature range (K), min.	620.92
Temperature range (K), max.	786.64

Sources

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C502738&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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