

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)CCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	450.82
CAS:	502-73-8

Physical Properties

Property code	Value	Unit	Source
gf	81.22	kJ/mol	Joback Method
hf	-795.75	kJ/mol	Joback Method
hfus	77.65	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	11.518		Crippen Method
mvol	449.220	ml/mol	McGowan Method
pc	585.99	kPa	Joback Method
rinpol	3304.20		NIST Webbook
rinpol	3304.20		NIST Webbook
tb	962.55	K	Joback Method
tc	1197.11	K	Joback Method
tf	356.40 ± 0.50	K	NIST Webbook
vc	1.778	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1581.38	J/mol×K	962.55	Joback Method

cpg	1608.78	J/molxK	1001.64	Joback Method
cpg	1634.36	J/molxK	1040.74	Joback Method
cpg	1658.24	J/molxK	1079.83	Joback Method
cpg	1680.55	J/molxK	1118.92	Joback Method
cpg	1701.41	J/molxK	1158.02	Joback Method
cpg	1720.95	J/molxK	1197.11	Joback Method
dvisc	0.0006463	Paxs	489.06	Joback Method
dvisc	0.0002408	Paxs	567.98	Joback Method
dvisc	0.0001141	Paxs	646.89	Joback Method
dvisc	0.0000636	Paxs	725.80	Joback Method
dvisc	0.0000398	Paxs	804.72	Joback Method
dvisc	0.0000271	Paxs	883.63	Joback Method
dvisc	0.0000196	Paxs	962.55	Joback Method
hfust	117.10	kJ/mol	356.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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=C502738&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
mccvol:	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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