

Hexacosanoic acid

Other names:	Ceratinic acid Ceric acid Cerinic acid Cerotic acid Hexacosanic acid
Inchi:	InChI=1S/C26H52O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24
InchiKey:	XMHIUKTWLZUKEX-UHFFFAOYSA-N
Formula:	C26H52O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	396.69
CAS:	506-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-97.70	kJ/mol	Joback Method
hf	-844.78	kJ/mol	Joback Method
hfus	68.78	kJ/mol	Joback Method
hvap	96.89	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.453		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	789.49	kPa	Joback Method
tb	940.33	K	Joback Method
tc	1164.73	K	Joback Method
tf	359.45 ± 2.00	K	NIST Webbook
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.38	J/mol×K	940.33	Joback Method
cpg	1355.39	J/mol×K	977.73	Joback Method
cpg	1376.92	J/mol×K	1015.13	Joback Method
cpg	1397.08	J/mol×K	1052.53	Joback Method

cpg	1415.96	J/mol×K	1089.93	Joback Method
cpg	1433.65	J/mol×K	1127.33	Joback Method
cpg	1450.25	J/mol×K	1164.73	Joback Method
dvisc	0.0005271	Pa×s	493.53	Joback Method
dvisc	0.0001503	Pa×s	568.00	Joback Method
dvisc	0.0000573	Pa×s	642.46	Joback Method
dvisc	0.0000267	Pa×s	716.93	Joback Method
dvisc	0.0000144	Pa×s	791.40	Joback Method
dvisc	0.0000086	Pa×s	865.86	Joback Method
dvisc	0.0000056	Pa×s	940.33	Joback Method
hvapt	177.20	kJ/mol	298.15	Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.30137e+01
Coeff. B	-1.03256e+04
Coeff. C	-1.61368e+02
Temperature range (K), min.	615.72
Temperature range (K), max.	744.67

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=C506467&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
Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je5009729

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

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