Tetracosanoic acid

Other names: Lignoceric acid
Inchi: InChI=1S/C24H48O2/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: QZZGJDVWLFXDLK-UHFFFAOYSA-N
Formula: C24H48O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 368.64
CAS: 557-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-114.54	kJ/mol	Joback Method
hf	-803.50	kJ/mol	Joback Method
hfus	63.60	kJ/mol	Joback Method
hvap	92.44	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.673		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	882.09	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2685.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	894.57	K	Joback Method
tc	1099.97	K	Joback Method
tf	358.45 ± 2.00	K	NIST Webbook
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.61	J/mol×K	1099.97	Joback Method
cpg	1297.99	J/mol×K	1065.74	Joback Method
cpg	1281.39	J/mol×K	1031.50	Joback Method
cpg	1263.76	J/mol×K	997.27	Joback Method

cpg	1245.02	J/mol×K	963.04	Joback Method
cpg	1225.12	J/mol×K	928.80	Joback Method
cpg	1203.98	J/mol×K	894.57	Joback Method
dvisc	0.0007730	Pa×s	470.99	Joback Method
dvisc	0.0000081	Pa×s	894.57	Joback Method
dvisc	0.0000125	Pa×s	823.97	Joback Method
dvisc	0.0000209	Pa×s	753.38	Joback Method
dvisc	0.0000390	Pa×s	682.78	Joback Method
dvisc	0.0000838	Pa×s	612.18	Joback Method
dvisc	0.0002203	Pa×s	541.59	Joback Method
hvapt	170.70	kJ/mol	298.15	Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	545.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.12110e+01
Coeff. B	-9.15711e+03
Coeff. C	-1.52472e+02
Temperature range (K), min.	590.12
Temperature range (K), max.	728.41

Sources

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
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=C557595&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume