Docosanoic acid

Other names:	1-Docosanoic acid
	Behenic acid
	Glycon B-70
	Hydrofol 2022-55
	Hydrofol Acid 560
	Hystrene 5522
	Hystrene 9022
	Prifrac 2989
	n-Docosanoic acid
Inchi:	InChI=1S/C22H44O2/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:	UKMSUNONTOPOIO-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	340.58
CAS:	112-85-6

Physical Properties

Property code	Value	Unit	Source
gf	-131.38	kJ/mol	Joback Method
hf	-762.22	kJ/mol	Joback Method
hfus	58.42	kJ/mol	Joback Method
hvap	87.99	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.893		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	848.81	K	Joback Method
tc	1039.78	K	Joback Method
tf	353.20 ± 1.50	K	NIST Webbook

tt	340.90	K	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.63	J/mol×K	1039.78	Joback Method
cpg	1078.06	J/mol×K	848.81	Joback Method
cpg	1097.63	J/mol×K	880.64	Joback Method
cpg	1116.14	J/mol×K	912.47	Joback Method
cpg	1133.65	J/mol×K	944.30	Joback Method
cpg	1150.20	J/mol×K	976.12	Joback Method
cpg	1165.85	J/mol×K	1007.95	Joback Method
dvisc	0.0000117	Pa×s	848.81	Joback Method
dvisc	0.0011337	Pa×s	448.45	Joback Method
dvisc	0.0003230	Pa×s	515.18	Joback Method
dvisc	0.0001227	Pa×s	581.90	Joback Method
dvisc	0.0000569	Pa×s	648.63	Joback Method
dvisc	0.0000304	Pa×s	715.36	Joback Method
dvisc	0.0000181	Pa×s	782.08	Joback Method
hsubt	193.00 ± 7.90	kJ/mol	344.60	NIST Webbook
hvapt	122.30	kJ/mol	486.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.97490e+01
Coeff. B	-8.19218e+03
Coeff. C	-1.43576e+02
Temperature range (K), min.	564.52
Temperature range (K), max.	711.00

Sources

Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Phase Equilibria of Long-Chain Carboxylic Acids in Supercritical Propane:	https://www.doi.org/10.1021/je101077v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Physical properties of systems of interest to the edible oil industry:	https://www.doi.org/10.1016/j.jct.2017.06.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent):	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	

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
hsubt:	Enthalpy of sublimation at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume