

Erucic acid

Other names:	(13Z)-13-docosenoic acid (Z)-13-Docosenoic acid (Z)-docos-13-enoic acid 13-Docosenoic acid, (Z)- 13-docosenoic acid (Z) Prifrac 2990 cis-13-Docosenoic acid «delta» 13-cis-Docosenoic acid Â«deltaÂ» 13-cis-Docosenoic acid
Inchi:	InChI=1S/C22H42O2/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:	DPUOLQHDNGRHBS-KTKRTIGZSA-N
Formula:	C22H42O2
SMILES:	CCCCCCCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	338.57
CAS:	112-86-7

Physical Properties

Property code	Value	Unit	Source
gf	-51.16	kJ/mol	Joback Method
hf	-645.00	kJ/mol	Joback Method
hfus	58.62	kJ/mol	Joback Method
hvap	87.95	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.669		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
tb	852.97	K	Joback Method
tc	1044.39	K	Joback Method
tf	443.37	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	1137.36	J/molxK	1012.49	Joback Method
cpg	1105.83	J/molxK	948.68	Joback Method
cpg	1088.82	J/molxK	916.78	Joback Method
cpg	1070.89	J/molxK	884.87	Joback Method
cpg	1052.00	J/molxK	852.97	Joback Method
cpg	1121.99	J/molxK	980.59	Joback Method
cpg	1152.00	J/molxK	1044.39	Joback Method
dvisc	0.0010953	Paxs	443.37	Joback Method
dvisc	0.0000101	Paxs	852.97	Joback Method
dvisc	0.0000157	Paxs	784.70	Joback Method
dvisc	0.0000266	Paxs	716.44	Joback Method
dvisc	0.0000503	Paxs	648.17	Joback Method
dvisc	0.0001102	Paxs	579.90	Joback Method
dvisc	0.0002981	Paxs	511.64	Joback Method
hfust	54.00	kJ/mol	307.20	NIST Webbook
hvapt	98.20	kJ/mol	567.00	NIST Webbook
hvapt	154.50	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	631.20	K	53.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66104e+01
Coeff. B	-6.84544e+03
Coeff. C	-1.42742e+02
Temperature range (K), min.	562.12
Temperature range (K), max.	748.59

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=C112867&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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