(E)-13-Docosenoic acid

Other names: (E)-docos-13-enoic acid
13-Docosenoic acid, (E)-
Brassidic acid
trans-13-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-MDZDMXLPSA-N
Formula: C22H42O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 338.57
CAS: 506-33-2

Physical Properties

Property code	Value	Unit	Source
chs	-13699.00 ± 2.70	kJ/mol	NIST Webbook
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
cpg	1152.00	J/mol×K	1044.39	Joback Method
cpg	1137.36	J/mol×K	1012.49	Joback Method
cpg	1121.99	J/mol×K	980.59	Joback Method
cpg	1105.83	J/mol×K	948.68	Joback Method

cpg	1088.82	J/mol×K	916.78	Joback Method
cpg	1070.89	J/mol×K	884.87	Joback Method
cpg	1052.00	J/mol×K	852.97	Joback Method
dvisc	0.0010953	Pa×s	443.37	Joback Method
dvisc	0.0000101	Pa×s	852.97	Joback Method
dvisc	0.0000157	Pa×s	784.70	Joback Method
dvisc	0.0000266	Pa×s	716.44	Joback Method
dvisc	0.0000503	Pa×s	648.17	Joback Method
dvisc	0.0001102	Pa×s	579.90	Joback Method
dvisc	0.0002981	Pa×s	511.64	Joback Method
hvapt	103.40	kJ/mol	569.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	555.20	K	4.00	NIST Webbook
tbrp	529.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C506332&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume