Docosanoic acid, ethyl ester

Other names:	Ethyl behenoate
	Ethyl docosanoate
Inchi:	InChI=1S/C24H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(25
InchiKey:	JIZCYLOUIAIZHQ-UHFFFAOYSA-N
Formula:	C24H48O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	368.64
CAS:	5908-87-2

Physical Properties

Property code	Value	Unit	Source
chs	-15196.00 ± 1.00	kJ/mol	NIST Webbook
gf	-82.72	kJ/mol	Joback Method
hf	-783.49	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.371		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2576.00		NIST Webbook
rinpol	2593.50		NIST Webbook
rinpol	2593.50		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2576.00		NIST Webbook
ripol	2883.00		NIST Webbook
ripol	2883.00		NIST Webbook
tb	824.81	K	Joback Method
tc	1009.81	K	Joback Method
tf	432.40	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.08	J/mol×K	1009.81	Joback Method
cpg	1156.81	J/mol×K	824.81	Joback Method
cpg	1178.47	J/mol×K	855.64	Joback Method
cpg	1198.97	J/mol×K	886.48	Joback Method
cpg	1218.34	J/mol×K	917.31	Joback Method
cpg	1236.63	J/mol×K	948.14	Joback Method
cpg	1253.86	J/mol×K	978.97	Joback Method
dvisc	0.0000418	Pa×s	824.81	Joback Method
dvisc	0.0010603	Pa×s	432.40	Joback Method
dvisc	0.0004342	Pa×s	497.80	Joback Method
dvisc	0.0002188	Pa×s	563.20	Joback Method
dvisc	0.0001271	Pa×s	628.61	Joback Method
dvisc	0.0000818	Pa×s	694.01	Joback Method
dvisc	0.0000568	Pa×s	759.41	Joback Method
hfust	77.82	kJ/mol	321.00	NIST Webbook
hfust	19.16	kJ/mol	321.00	NIST Webbook
hsubt	196.50	kJ/mol	315.50	NIST Webbook
hvapt	127.50	kJ/mol	335.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	514.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.91277e+01
Coeff. B	-1.24178e+04
Coeff. C	-1.65424e+02

Temperature range (K), min.	596.00
Temperature range (K), max.	686.82

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5908872&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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	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