(E,E)-2,13-octadecadienal

Inchi: InChI=1S/C18H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h5-6,16-18H,2-4
InchiKey: NCFULMZVHNTQOK-JNHUCFJMSA-N
Formula: C18H32O
SMILES: CCCCC=CCCCCCCCCCC=CC=O
Mol. weight [g/mol]: 264.45

Physical Properties

Property code	Value	Unit	Source
gf	161.60	kJ/mol	Joback Method
hf	-265.99	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.999		Crippen Method
mcvol	257.450	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	668.22	K	Joback Method
tc	841.93	K	Joback Method
tf	324.46	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.37	J/mol×K	668.22	Joback Method
cpg	795.94	J/mol×K	812.98	Joback Method
cpg	781.12	J/mol×K	784.03	Joback Method
cpg	765.60	J/mol×K	755.08	Joback Method
cpg	749.33	J/mol×K	726.12	Joback Method
cpg	732.27	J/mol×K	697.17	Joback Method
cpg	810.09	J/mol×K	841.93	Joback Method
dvisc	0.0001016	Pa×s	668.22	Joback Method

dvisc	0.0001374	Pa×s	610.93	Joback Method
dvisc	0.0001978	Pa×s	553.63	Joback Method
dvisc	0.0003097	Pa×s	496.34	Joback Method
dvisc	0.0005452	Pa×s	439.05	Joback Method
dvisc	0.0011371	Pa×s	381.75	Joback Method
dvisc	0.0030745	Pa×s	324.46	Joback Method

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=R399143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume