cis-13-Eicosenoic acid

Other names: (Z)-13-Eicosenic acid
Inchi: InChI=1S/C20H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h7-8H
InchiKey: URXZXNYJPAJJOQ-FPLPWBNLSA-N
Formula: C20H38O2
SMILES: CCCCCCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 310.51
CAS: 17735-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-68.00	kJ/mol	Joback Method
hf	-603.72	kJ/mol	Joback Method
hfus	53.45	kJ/mol	Joback Method
hvap	83.50	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.889		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2365.50		NIST Webbook
rinpol	2365.50		NIST Webbook
tb	807.21	K	Joback Method
tc	989.21	K	Joback Method
tf	420.83	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.92	J/mol×K	807.21	Joback Method
cpg	1009.77	J/mol×K	958.87	Joback Method
cpg	995.34	J/mol×K	928.54	Joback Method
cpg	980.19	J/mol×K	898.21	Joback Method
cpg	964.26	J/mol×K	867.88	Joback Method
cpg	947.52	J/mol×K	837.54	Joback Method

cpg	1023.52	J/mol×K	989.21	Joback Method
dvisc	0.0000146	Pa×s	807.21	Joback Method
dvisc	0.0000228	Pa×s	742.81	Joback Method
dvisc	0.0000386	Pa×s	678.42	Joback Method
dvisc	0.0000732	Pa×s	614.02	Joback Method
dvisc	0.0001611	Pa×s	549.62	Joback Method
dvisc	0.0004374	Pa×s	485.23	Joback Method
dvisc	0.0016119	Pa×s	420.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17735943&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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