8,11,14-Eicosatrienoic acid, (Z,Z,Z)-

Other names: cis-8,11,14-Eicosatrienoic Acid
Dihomo-«gamma»-linolenic acid
(Z,Z,Z)-icosatri-8,11,14-enoic acid
Inchi: InChI=1S/C20H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h6-7,
InchiKey: HOBAELRKJCKHQD-YHTMAJSVSA-N
Formula: C20H34O2
SMILES: CCCCCC=CCC=CCC=CCCCCCCC(=O)O
Mol. weight [g/mol]: 306.48
CAS: 1783-84-2

Physical Properties

Property code	Value	Unit	Source
gf	92.44	kJ/mol	Joback Method
hf	-369.28	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	83.41	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.441		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2345.90		NIST Webbook
rinpol	2345.90		NIST Webbook
tb	815.53	K	Joback Method
tc	1001.77	K	Joback Method
tf	410.67	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.04	J/mol×K	815.53	Joback Method
cpg	895.49	J/mol×K	846.57	Joback Method
cpg	911.19	J/mol×K	877.61	Joback Method
cpg	926.21	J/mol×K	908.65	Joback Method

cpg	940.62	J/mol×K	939.69	Joback Method
cpg	954.47	J/mol×K	970.73	Joback Method
cpg	967.84	J/mol×K	1001.77	Joback Method
dvisc	0.0015216	Pa×s	410.67	Joback Method
dvisc	0.0003734	Pa×s	478.15	Joback Method
dvisc	0.0001297	Pa×s	545.62	Joback Method
dvisc	0.0000569	Pa×s	613.10	Joback Method
dvisc	0.0000294	Pa×s	680.58	Joback Method
dvisc	0.0000171	Pa×s	748.05	Joback Method
dvisc	0.0000109	Pa×s	815.53	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1783842&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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