Eicosanal

Other names:	1-Eicosanal
	icosanal
Inchi:	InChI=1S/C20H40O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h20H,2-19
InchiKey:	FWBUWJHWAKTPHI-UHFFFAOYSA-N
Formula:	C20H40O
SMILES:	CCCCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]:	296.53
CAS:	2400-66-0

Physical Properties

Property code	Value	Unit	Source
gf	18.00	kJ/mol	Joback Method
hf	-541.71	kJ/mol	Joback Method
hfus	49.84	kJ/mol	Joback Method
hvap	66.83	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.227		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2203.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	2224.00		NIST Webbook
rinpol	2225.30		NIST Webbook
rinpol	2219.00		NIST Webbook
ripol	2571.00		NIST Webbook
tb	705.66	K	Joback Method
tc	872.64	K	Joback Method
tf	357.16	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.08	J/mol×K	705.66	Joback Method
cpg	963.88	J/mol×K	844.81	Joback Method
cpg	947.55	J/mol×K	816.98	Joback Method
cpg	930.43	J/mol×K	789.15	Joback Method
cpg	912.50	J/mol×K	761.32	Joback Method
cpg	893.73	J/mol×K	733.49	Joback Method
cpg	979.46	J/mol×K	872.64	Joback Method
dvisc	0.0001071	Pa×s	705.66	Joback Method
dvisc	0.0001450	Pa×s	647.58	Joback Method
dvisc	0.0002084	Pa×s	589.49	Joback Method
dvisc	0.0003245	Pa×s	531.41	Joback Method
dvisc	0.0005629	Pa×s	473.33	Joback Method
dvisc	0.0011395	Pa×s	415.24	Joback Method
dvisc	0.0029013	Pa×s	357.16	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=C2400660&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume