

(Z)-Icos-9-enoic 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/h11-1
InchiKey:	LQJBNNIYVWPHFW-QXMHVHEDSA-N
Formula:	C20H38O2
SMILES:	CCCCCCCCC=CCCCCCCC(=O)O
Mol. weight [g/mol]:	310.51
CAS:	29204-02-2

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	2338.50		NIST Webbook
rinpol	2338.50		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/molxK	807.21	Joback Method
cpg	947.52	J/molxK	837.54	Joback Method
cpg	964.26	J/molxK	867.88	Joback Method
cpg	980.19	J/molxK	898.21	Joback Method
cpg	995.34	J/molxK	928.54	Joback Method
cpg	1009.77	J/molxK	958.87	Joback Method
cpg	1023.52	J/molxK	989.21	Joback Method

dvisc	0.0016119	Paxs	420.83	Joback Method
dvisc	0.0004374	Paxs	485.23	Joback Method
dvisc	0.0001611	Paxs	549.62	Joback Method
dvisc	0.0000732	Paxs	614.02	Joback Method
dvisc	0.0000386	Paxs	678.42	Joback Method
dvisc	0.0000228	Paxs	742.81	Joback Method
dvisc	0.0000146	Paxs	807.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C29204022&Units=SI

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
mvol:	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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