

8,11,14-Eicosatrienoic 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-QNEBEIHSSA-N
Formula:	C20H34O2
SMILES:	CCCCC=CCC=CC=CCCCCCC(=O)O
Mol. weight [g/mol]:	306.48
CAS:	7324-41-6

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	2135.00		NIST Webbook
tb	815.53	K	Joback Method
tc	1001.77	K	Joback Method
tf	410.67	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.04	J/molxK	815.53	Joback Method
cpg	895.49	J/molxK	846.57	Joback Method
cpg	911.19	J/molxK	877.61	Joback Method
cpg	926.21	J/molxK	908.65	Joback Method
cpg	940.62	J/molxK	939.69	Joback Method
cpg	954.47	J/molxK	970.73	Joback Method
cpg	967.84	J/molxK	1001.77	Joback Method
dvisc	0.0015216	Paxs	410.67	Joback Method

dvisc	0.0003734	Paxs	478.15	Joback Method
dvisc	0.0001297	Paxs	545.62	Joback Method
dvisc	0.0000569	Paxs	613.10	Joback Method
dvisc	0.0000294	Paxs	680.58	Joback Method
dvisc	0.0000171	Paxs	748.05	Joback Method
dvisc	0.0000109	Paxs	815.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7324416&Units=SI
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

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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