

(Z)-9-(E)-12-Tetradecadienal

Inchi:	InChI=1S/C14H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h2-3,5-6,14H,4,7-13H2,1H3/b
InchiKey:	XHXSPBYEQUMCKE-OHAITUNLSA-N
Formula:	C14H24O
SMILES:	CC=CCC=CCCCCCCCC=O
Mol. weight [g/mol]:	208.34

Physical Properties

Property code	Value	Unit	Source
gf	127.92	kJ/mol	Joback Method
hf	-183.43	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.438		Crippen Method
mcvol	201.090	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2053.00		NIST Webbook
tb	576.70	K	Joback Method
tc	753.90	K	Joback Method
tf	279.38	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.57	J/molxK	576.70	Joback Method
cpg	515.69	J/molxK	606.23	Joback Method
cpg	531.04	J/molxK	635.77	Joback Method
cpg	545.64	J/molxK	665.30	Joback Method
cpg	559.54	J/molxK	694.83	Joback Method
cpg	572.78	J/molxK	724.36	Joback Method

cpg	585.38	J/mol×K	753.90	Joback Method
dvisc	0.0040632	Paxs	279.38	Joback Method
dvisc	0.0015613	Paxs	328.93	Joback Method
dvisc	0.0007707	Paxs	378.49	Joback Method
dvisc	0.0004480	Paxs	428.04	Joback Method
dvisc	0.0002914	Paxs	477.59	Joback Method
dvisc	0.0002055	Paxs	527.15	Joback Method
dvisc	0.0001539	Paxs	576.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554820&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

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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