

(E,E,E)-2,4,6-tetradecatrienal

Inchi:	InChI=1S/C14H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h8-14H,2-7H2,1H3/b9-8+,11-
InchiKey:	MHJQZJXVYHMAAZ-GTEMLCSVSA-N
Formula:	C14H22O
SMILES:	CCCCCCCC=CC=CC=CC=O
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	208.14	kJ/mol	Joback Method
hf	-66.21	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.214		Crippen Method
mcvol	196.790	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	580.86	K	Joback Method
tc	764.94	K	Joback Method
tf	274.30	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.34	J/molxK	580.86	Joback Method
cpg	551.16	J/molxK	734.26	Joback Method
cpg	538.45	J/molxK	703.58	Joback Method
cpg	525.06	J/molxK	672.90	Joback Method
cpg	510.95	J/molxK	642.22	Joback Method
cpg	496.06	J/molxK	611.54	Joback Method
cpg	563.25	J/molxK	764.94	Joback Method
dvisc	0.0001313	Paxs	580.86	Joback Method

dvisc	0.0001756	Paxs	529.77	Joback Method
dvisc	0.0002499	Paxs	478.67	Joback Method
dvisc	0.0003868	Paxs	427.58	Joback Method
dvisc	0.0006740	Paxs	376.49	Joback Method
dvisc	0.0013985	Paxs	325.39	Joback Method
dvisc	0.0038084	Paxs	274.30	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=R236978&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
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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