

(E,E,Z)-2,4,7-tridecatrienal

Inchi:	InChI=1S/C13H20O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h6-7,9-13H,2-5,8H2,1H3/b7-6-,1
InchiKey:	BIXIZZVISIZZDM-DFHZKIAOSA-N
Formula:	C13H20O
SMILES:	CCCCC=CCC=CC=CC=O
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	199.72	kJ/mol	Joback Method
hf	-45.57	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinsol	1630.00		NIST Webbook
tb	557.98	K	Joback Method
tc	744.04	K	Joback Method
tf	263.03	K	Joback Method
vc	0.721	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.82	J/molxK	557.98	Joback Method
cpg	445.98	J/molxK	588.99	Joback Method
cpg	460.33	J/molxK	620.00	Joback Method
cpg	473.90	J/molxK	651.01	Joback Method
cpg	486.76	J/molxK	682.02	Joback Method
cpg	498.94	J/molxK	713.03	Joback Method
cpg	510.51	J/molxK	744.04	Joback Method
dvisc	0.0039796	Paxs	263.03	Joback Method
dvisc	0.0014768	Paxs	312.19	Joback Method

dvisc	0.0007177	Paxs	361.35	Joback Method
dvisc	0.0004146	Paxs	410.50	Joback Method
dvisc	0.0002693	Paxs	459.66	Joback Method
dvisc	0.0001902	Paxs	508.82	Joback Method
dvisc	0.0001428	Paxs	557.98	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=R237055&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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<https://www.chemeo.com/cid/49-482-3/E-E-Z-2-4-7-tridecatrienal.pdf>

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