

1-(E,Z,Z)-3,5,8-undecatetraene

Inchi:	InChI=1S/C11H16/c1-3-5-7-9-11-10-8-6-4-2/h3,5-9,11H,1,4,10H2,2H3/b7-5+,8-6-,11-9-
InchiKey:	JXRWPVZILDJGFO-PWYDJTSCSA-N
Formula:	C11H16
SMILES:	C=CC=CC=CCC=CCC
Mol. weight [g/mol]:	148.24

Physical Properties

Property code	Value	Unit	Source
gf	370.24	kJ/mol	Joback Method
hf	206.72	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	39.28	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.641		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1449.00		NIST Webbook
tb	460.24	K	Joback Method
tc	649.54	K	Joback Method
tf	196.73	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.88	J/mol×K	460.24	Joback Method
cpg	310.73	J/mol×K	491.79	Joback Method
cpg	324.71	J/mol×K	523.34	Joback Method
cpg	337.87	J/mol×K	554.89	Joback Method
cpg	350.26	J/mol×K	586.44	Joback Method

cpg	361.95	J/mol×K	617.99	Joback Method
cpg	372.97	J/mol×K	649.54	Joback Method
dvisc	0.0044996	Pa×s	196.73	Joback Method
dvisc	0.0014648	Pa×s	240.65	Joback Method
dvisc	0.0006743	Pa×s	284.57	Joback Method
dvisc	0.0003819	Pa×s	328.49	Joback Method
dvisc	0.0002474	Pa×s	372.40	Joback Method
dvisc	0.0001756	Pa×s	416.32	Joback Method
dvisc	0.0001331	Pa×s	460.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R168573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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