

1,3,5,8-Undecatetraene

Other names:	1,3,5,8-Undecatetraene, (E,E,Z)- (E,E,Z)-undeca-1,3,5,8-tetraene
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-NDNIUKBNSA-N
Formula:	C11H16
SMILES:	C=CC=CC=CCC=CCC
Mol. weight [g/mol]:	148.24
CAS:	50277-31-1

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	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1177.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1454.00		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=C50277311&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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