

1-Tridecene-3,5,7,9,11-pentayne

Other names:	1-Tridecen-3,5,7,9,11-pentayne
Inchi:	InChI=1S/C13H6/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3H,1H2,2H3
InchiKey:	KKBHBCOJHHCOCL-UHFFFAOYSA-N
Formula:	C13H6
SMILES:	C=CC#CC#CC#CC#CC
Mol. weight [g/mol]:	162.19

Physical Properties

Property code	Value	Unit	Source
gf	1160.42	kJ/mol	Joback Method
hf	1175.28	kJ/mol	Joback Method
hfus	43.76	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	1.209		Crippen Method
mcvol	146.730	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	1780.00		NIST Webbook
tb	538.52	K	Joback Method
tc	845.59	K	Joback Method
tf	765.01	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.37	J/mol×K	538.52	Joback Method
cpg	278.96	J/mol×K	589.70	Joback Method
cpg	290.78	J/mol×K	640.88	Joback Method
cpg	301.88	J/mol×K	692.05	Joback Method
cpg	312.30	J/mol×K	743.23	Joback Method
cpg	322.08	J/mol×K	794.41	Joback Method
cpg	331.27	J/mol×K	845.59	Joback Method

Sources

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=R54620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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