(Z,E)-1,3,11-tridecatriene-5,7,9-triyne

Other names:	(Z,E)-1,3,11-Tridecatrien-5,7,9-triyne
	1,3(Z),11(E)-Tridecatrien-5,7,9-triyne
Inchi:	InChI=1S/C13H10/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-7H,1H2,2H3/b6-4+,7-5-
InchiKey:	KAGUESUDHDXNCN-GUBXDBFYSA-N
Formula:	C13H10
SMILES:	C=CC=CC#CC#CC#CC=CC
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	915.26	kJ/mol	Joback Method
hf	865.12	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.315		Crippen Method
mcvol	155.330	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook
tb	528.84	K	Joback Method
tc	787.02	K	Joback Method
tf	542.65	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	301.84	J/mol×K	528.84	Joback Method
cpg	315.90	J/mol×K	571.87	Joback Method
cpg	328.98	J/mol×K	614.90	Joback Method
cpg	341.16	J/mol×K	657.93	Joback Method
cpg	352.54	J/mol×K	700.96	Joback Method
cpg	363.21	J/mol×K	743.99	Joback Method
cpg	373.25	J/mol×K	787.02	Joback Method

Sources

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=R54787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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