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

Inchi: InChI=1S/C13H10/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3,5,7,9,11H,1H2,2H3/b7-5+,11-9-
InchiKey: AJWRNFIZKHPOHC-STRRHFTISA-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	1687.00		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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54705&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume