(Z,E,E)-1,3,5,11-Tridecatetraene-7,9-diyne

Inchi: InChI=1S/C13H12/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-7,9,11H,1H2,2H3/b6-4+,7-5-,11-9+

InchiKey: ASVIELUINMCNMW-GIDTTZPASA-N

Formula: C13H12

SMILES: C=CC=CC=CC#CC#CC=CC

Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	792.68	kJ/mol	Joback Method
hf	710.04	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	48.04	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	2.868		Crippen Method
mcvol	159.630	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1650.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2310.00		NIST Webbook
tb	524.00	K	Joback Method
tc	761.55	K	Joback Method
tf	431.47	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.96	J/mol×K	524.00	Joback Method
cpg	333.60	J/mol×K	563.59	Joback Method
cpg	347.20	J/mol×K	603.18	Joback Method
cpg	359.85	J/mol×K	642.78	Joback Method
cpg	371.66	J/mol×K	682.37	Joback Method
cpg	382.72	J/mol×K	721.96	Joback Method

cpg	393.13	J/mol×K	761.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54791&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
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