1,3,5,7-Tridecatetraene-7,9-diyne isomer # 1

Other names: 1,3(E),5(E),11(E)-Tridecatetraen-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-FSNIPRKGSA-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	1648.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
ripol	2405.00		NIST Webbook
ripol	2405.00		NIST Webbook
ripol	2405.00		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

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=R54616&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume