

(E)-1,11-Tridecadiene-3,5,7,9-tetrayne

Other names:	1,11(E)-Tridecadien-3,5,7,9-tetrayne
Inchi:	InChI=1S/C13H8/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-4,6H,1H2,2H3/b6-4+
InchiKey:	KBEMPFYJJCTZIG-GQCTYLIASA-N
Formula:	C13H8
SMILES:	C=CC#CC#CC#CC#CC=CC
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
gf	1037.84	kJ/mol	Joback Method
hf	1020.20	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	1.762		Crippen Method
mcvol	151.030	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1712.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2484.00		NIST Webbook
tb	533.68	K	Joback Method
tc	814.93	K	Joback Method
tf	653.83	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.30	J/mol×K	533.68	Joback Method
cpg	297.69	J/mol×K	580.55	Joback Method

cpg	310.18	J/mol×K	627.43	Joback Method
cpg	321.85	J/mol×K	674.30	Joback Method
cpg	332.76	J/mol×K	721.18	Joback Method
cpg	343.00	J/mol×K	768.05	Joback Method
cpg	352.65	J/mol×K	814.93	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=R54652&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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