

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

Inchi: InChI=1S/C13H8/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3,5,7H,1H2,2H3/b7-5+
InchiKey: PXQLZFYDZKYLPY-FNORWQNLSA-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	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
ripol	2277.00		NIST Webbook
tb	533.68	K	Joback Method
tc	814.93	K	Joback Method
tf	653.83	K	Joback Method
vc	0.573	m ³ /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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R54666&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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