(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=C/C=C/C#CC#CC#CC#CC
Mol. weight [g/mol]: 164.21

Physical Properties

Property code	Value	Unit	Source
hfus	40.84	kJ/mol	Joback Method
logp	1.762		Crippen Method
mcvol	151.030	ml/mol	McGowan Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2277.00		NIST Webbook

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54666&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices