

1-Phenyl-2,4-pentadiyne

Inchi:	InChI=1S/C11H12/c1-2-3-5-8-11-9-6-4-7-10-11/h2-7,9-10H,1,8H2/b5-3+
InchiKey:	XIKDQDXWYVAHNF-HWKANZROSA-N
Formula:	C11H12
SMILES:	C=CC=CCc1ccccc1
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	322.21	kJ/mol	Joback Method
hf	208.81	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	41.64	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.971		Crippen Method
mcvol	133.490	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
tb	478.60	K	Joback Method
tc	695.21	K	Joback Method
tf	233.31	K	Joback Method
vc	0.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.82	J/mol×K	478.60	Joback Method
cpg	280.90	J/mol×K	514.70	Joback Method
cpg	294.97	J/mol×K	550.80	Joback Method
cpg	308.08	J/mol×K	586.90	Joback Method
cpg	320.30	J/mol×K	623.01	Joback Method
cpg	331.68	J/mol×K	659.11	Joback Method
cpg	342.29	J/mol×K	695.21	Joback Method
dvisc	0.0031494	Paxs	233.31	Joback Method

dvisc	0.0013804	Paxs	274.19	Joback Method
dvisc	0.0007494	Paxs	315.07	Joback Method
dvisc	0.0004682	Paxs	355.96	Joback Method
dvisc	0.0003222	Paxs	396.84	Joback Method
dvisc	0.0002378	Paxs	437.72	Joback Method
dvisc	0.0001849	Paxs	478.60	Joback Method

Sources

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=R333836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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