

1-Phenyl-2,4-pentadiynone

Inchi:	InChI=1S/C11H10O/c1-2-3-9-11(12)10-7-5-4-6-8-10/h2-9H,1H2/b9-3+
InchiKey:	VQMPPKIHOBTTQQK-YCRREMRBSA-N
Formula:	C11H10O
SMILES:	C=CC=CC(=O)c1ccccc1
Mol. weight [g/mol]:	158.20

Physical Properties

Property code	Value	Unit	Source
gf	193.29	kJ/mol	Joback Method
hf	96.23	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.612		Crippen Method
mcvol	135.060	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	532.47	K	Joback Method
tc	758.77	K	Joback Method
tf	283.24	K	Joback Method
vc	0.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.33	J/molxK	532.47	Joback Method
cpg	342.95	J/molxK	721.06	Joback Method
cpg	332.96	J/molxK	683.34	Joback Method
cpg	322.17	J/molxK	645.62	Joback Method
cpg	310.51	J/molxK	607.90	Joback Method
cpg	297.92	J/molxK	570.19	Joback Method
cpg	352.20	J/molxK	758.77	Joback Method
dvisc	0.0002108	Paxs	532.47	Joback Method

dvisc	0.0002691	Paxs	490.93	Joback Method
dvisc	0.0003593	Paxs	449.39	Joback Method
dvisc	0.0005091	Paxs	407.86	Joback Method
dvisc	0.0007805	Paxs	366.32	Joback Method
dvisc	0.0013347	Paxs	324.78	Joback Method
dvisc	0.0026717	Paxs	283.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R333841&Units=SI

Legend

cpg:	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:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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