2,4-Hexadiyn-1-one, 1-phenyl-

Other names: 2,4-Hexadiynophenone
Capillin
Inchi: InChI=1S/C12H8O/c1-2-3-5-10-12(13)11-8-6-4-7-9-11/h4,6-9H,1H3
InchiKey: RAZOKRUZEQERLH-UHFFFAOYSA-N
Formula: C12H8O
SMILES: CC#CC#CC(=O)c1ccccc1
Mol. weight [g/mol]: 168.19
CAS: 495-74-9

Physical Properties

Property code	Value	Unit	Source
gf	439.25	kJ/mol	Joback Method
hf	377.54	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	55.63	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	1.896		Crippen Method
mcvol	140.550	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	572.51	K	Joback Method
tc	839.40	K	Joback Method
tf	513.55	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.71	J/mol×K	572.51	Joback Method
cpg	306.32	J/mol×K	616.99	Joback Method
cpg	318.90	J/mol×K	661.47	Joback Method
cpg	330.50	J/mol×K	705.96	Joback Method

cpg	341.18	J/mol×K	750.44	Joback Method
cpg	351.00	J/mol×K	794.92	Joback Method
cpg	360.01	J/mol×K	839.40	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=C495749&Units=SI
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
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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