1-Phenylpenta-1-yn-3-one

Inchi: InChI=1S/C11H10O/c1-2-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2H2,1H3
InchiKey: XAJIQJSLJKBJTP-UHFFFAOYSA-N
Formula: C11H10O
SMILES: CCC(=O)C#Cc1ccccc1
Mol. weight [g/mol]: 158.20
CAS: 19307-74-5

Physical Properties

Property code	Value	Unit	Source
chl	-5804.90	kJ/mol	NIST Webbook
gf	228.03	kJ/mol	Joback Method
hf	125.88	kJ/mol	Joback Method
hfl	47.10 ± 5.00	kJ/mol	NIST Webbook
hfl	-9.20	kJ/mol	NIST Webbook
hfus	23.01	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.017		Crippen Method
mcvol	135.060	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	540.63	K	Joback Method
tc	780.40	K	Joback Method
tf	396.18	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.67	J/mol×K	540.63	Joback Method
cpg	299.49	J/mol×K	580.59	Joback Method
cpg	312.37	J/mol×K	620.55	Joback Method
cpg	324.35	J/mol×K	660.51	Joback Method
cpg	335.48	J/mol×K	700.48	Joback Method
cpg	345.80	J/mol×K	740.44	Joback Method

cpg	355.35	J/mol×K	780.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19307745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume