7-Phenylhept-4-yn-3-one

Inchi: InChI=1S/C13H14O/c1-2-13(14)11-7-6-10-12-8-4-3-5-9-12/h3-5,8-9H,2,6,10H2,1H3
InchiKey: RBBQVELPWQFPJO-UHFFFAOYSA-N
Formula: C13H14O
SMILES: CCC(=O)C#CCCc1ccccc1
Mol. weight [g/mol]: 186.25
CAS: 62059-60-3

Physical Properties

Property code	Value	Unit	Source
chl	-7064.70	kJ/mol	NIST Webbook
gf	244.87	kJ/mol	Joback Method
hf	84.60	kJ/mol	Joback Method
hfl	101.00	kJ/mol	NIST Webbook
hfl	-51.70 ± 6.00	kJ/mol	NIST Webbook
hfus	28.19	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.602		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	586.39	K	Joback Method
tc	816.75	K	Joback Method
tf	418.72	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.40	J/mol×K	586.39	Joback Method
cpg	393.90	J/mol×K	624.78	Joback Method
cpg	408.39	J/mol×K	663.18	Joback Method
cpg	421.92	J/mol×K	701.57	Joback Method
cpg	434.52	J/mol×K	739.96	Joback Method
cpg	446.26	J/mol×K	778.35	Joback Method

cpg	457.17	J/mol×K	816.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62059603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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