Tert-butyl(phenylacetylenyl)ketone

Inchi: InChI=1S/C13H14O/c1-13(2,3)12(14)10-9-11-7-5-4-6-8-11/h4-8H,1-3H3
InchiKey: QXGIWMOPVOXYCX-UHFFFAOYSA-N
Formula: C13H14O
SMILES: CC(C)(C)C(=O)C#Cc1ccccc1
Mol. weight [g/mol]: 186.25
CAS: 32398-67-7

Physical Properties

Property code	Value	Unit	Source
chl	-7115.40 ± 4.20	kJ/mol	NIST Webbook
gf	247.71	kJ/mol	Joback Method
hf	64.40 ± 4.20	kJ/mol	NIST Webbook
hf	64.60	kJ/mol	NIST Webbook
hfl	-1.30 ± 4.20	kJ/mol	NIST Webbook
hfl	-1.10 ± 4.60	kJ/mol	NIST Webbook
hfus	20.77	kJ/mol	Joback Method
hvap	65.70	kJ/mol	NIST Webbook
hvap	65.67	kJ/mol	NIST Webbook
log10ws	-3.30		Crippen Method
logp	2.653		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	402.00 ± 0.10	K	NIST Webbook
tc	828.62	K	Joback Method
tf	421.14	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.79	J/mol×K	583.16	Joback Method
cpg	398.25	J/mol×K	624.07	Joback Method
cpg	413.43	J/mol×K	664.98	Joback Method
cpg	427.42	J/mol×K	705.89	Joback Method

cpg	440.31	J/mol×K	746.80	Joback Method
cpg	452.19	J/mol×K	787.71	Joback Method
cpg	463.13	J/mol×K	828.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32398677&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

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