2-Cyclohexen-1-one, 4,4-diphenyl-

Other names: 4,4-Diphenyl-2-cyclohexen-1-one
Inchi: InChI=1S/C18H16O/c19-17-11-13-18(14-12-17,15-7-3-1-4-8-15)16-9-5-2-6-10-16/h1-11,
InchiKey: LUFGFXHHSGISSL-UHFFFAOYSA-N
Formula: C18H16O
SMILES: O=C1C=CC(c2ccccc2)(c2ccccc2)CC1
Mol. weight [g/mol]: 248.32
CAS: 4528-64-7

Physical Properties

Property code	Value	Unit	Source
gf	251.83	kJ/mol	Joback Method
hf	47.85	kJ/mol	Joback Method
hfus	16.73	kJ/mol	Joback Method
hvap	64.03	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.892		Crippen Method
mcvol	203.370	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	751.37	K	Joback Method
tc	1036.29	K	Joback Method
tf	445.72	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.99	J/mol×K	751.37	Joback Method
cpg	595.45	J/mol×K	798.86	Joback Method
cpg	614.61	J/mol×K	846.34	Joback Method
cpg	632.76	J/mol×K	893.83	Joback Method
cpg	650.19	J/mol×K	941.32	Joback Method
cpg	667.18	J/mol×K	988.80	Joback Method
cpg	684.02	J/mol×K	1036.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4528647&Units=SI

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