

Cyclohexanone, 6-methyl-2,2-diphenyl-

Inchi:	InChI=1S/C19H20O/c1-15-9-8-14-19(18(15)20,16-10-4-2-5-11-16)17-12-6-3-7-13-17/h2-
InchiKey:	KOTLGIFDJZDYEYV-UHFFFAOYSA-N
Formula:	C19H20O
SMILES:	CC1CCCC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]:	264.36
CAS:	50592-52-4

Physical Properties

Property code	Value	Unit	Source
gf	222.58	kJ/mol	Joback Method
hf	-50.91	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	65.66	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.362		Crippen Method
mcvol	221.760	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	770.42	K	Joback Method
tc	1045.75	K	Joback Method
tf	451.99	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.22	J/molxK	770.42	Joback Method
cpg	682.57	J/molxK	816.31	Joback Method
cpg	703.53	J/molxK	862.20	Joback Method
cpg	723.36	J/molxK	908.08	Joback Method
cpg	742.32	J/molxK	953.97	Joback Method
cpg	760.64	J/molxK	999.86	Joback Method
cpg	778.59	J/molxK	1045.75	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=C50592524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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