

Tetraphenylcyclopentadienone

Other names:	2,3,4,5-Tetraphenyl-2,4-cyclopentadienone 2,3,4,5-Tetraphenylcyclopentadienone Cyclone Cyclone (compound) NSC 2060 Tetracyclon Tetracyclone Tetraphenyl-2,4-cyclopentadien-1-one Tetraphenylcyclopentadienone
Inchi:	InChI=1S/C29H20O/c30-29-27(23-17-9-3-10-18-23)25(21-13-5-1-6-14-21)26(22-15-7-2-8-4-11-12-16-20-28-24-19-26)
InchiKey:	PLGPSDNOLCVGSS-UHFFFAOYSA-N
Formula:	C29H20O
SMILES:	O=C1C(c2ccccc2)=C(c2ccccc2)C(c2ccccc2)=C1c1ccccc1
Mol. weight [g/mol]:	384.48

Physical Properties

Property code	Value	Unit	Source
af	0.6487		Cheméo Relay (1.0)
gf	586.01	kJ/mol	Joback Method
hf	499.47	kJ/mol	Cheméo Relay (1.0)
hfus	40.29	kJ/mol	Joback Method
hvap	137.72	kJ/mol	Cheméo Relay (1.0)
ie	7.76	eV	Cheméo Relay (1.0)
log10ws	-7.62		Cheméo Relay (1.0)
logp	6.791		Crippen Method
mcvol	306.540	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
tb	769.12	K	Cheméo Relay (1.0)
tc	1148.35	K	Cheméo Relay (1.0)
tf	493.72	K	Cheméo Relay (1.0)
vc	1.088	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.31	J/mol×K	1075.65	Joback Method
cpg	977.89	J/mol×K	1124.48	Joback Method
cpg	988.98	J/mol×K	1173.31	Joback Method
cpg	998.78	J/mol×K	1222.14	Joback Method
cpg	1007.50	J/mol×K	1270.97	Joback Method
cpg	1015.35	J/mol×K	1319.79	Joback Method
cpg	1022.54	J/mol×K	1368.62	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479334&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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