2,4-Cyclopentadien-1-ol, 1,2,3,4,5-pentaphenyl-

Other names: Pentaphenylcyclopentadienol
Inchi: InChI=1S/C35H26O/c36-35(30-24-14-5-15-25-30)33(28-20-10-3-11-21-28)31(26-16-6-1-
InchiKey: DIFNJNDIHZLRLI-UHFFFAOYSA-N
Formula: C35H26O
SMILES: OC1(c2ccccc2)C(c2ccccc2)=C(c2ccccc2)C(c2ccccc2)=C1c1ccccc1
Mol. weight [g/mol]: 462.58
CAS: 2137-74-8

Physical Properties

Property code	Value	Unit	Source
gf	721.51	kJ/mol	Joback Method
hf	410.09	kJ/mol	Joback Method
hfus	49.22	kJ/mol	Joback Method
hvap	123.90	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	8.110		Crippen Method
mcvol	371.620	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
tb	1259.54	K	Joback Method
tc	1551.47	K	Joback Method
tf	763.53	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.07	J/mol×K	1259.54	Joback Method
cpg	1350.94	J/mol×K	1308.20	Joback Method
cpg	1387.95	J/mol×K	1356.85	Joback Method
cpg	1428.65	J/mol×K	1405.51	Joback Method
cpg	1473.57	J/mol×K	1454.16	Joback Method
cpg	1523.27	J/mol×K	1502.82	Joback Method
cpg	1578.29	J/mol×K	1551.47	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=C2137748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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