

Benzene, 1,1',1'',1''',1''''-(1,3-cyclopentadiene-1,2,3,4,5-penta

Inchi:	InChI=1S/C35H26/c1-6-16-26(17-7-1)31-32(27-18-8-2-9-19-27)34(29-22-12-4-13-23-29)
InchiKey:	YGLVWOUNCXBPJF-UHFFFAOYSA-N
Formula:	C35H26
SMILES:	c1ccc(C2=C(c3ccccc3)C(c3ccccc3)C(c3ccccc3)=C2c2ccccc2)cc1
Mol. weight [g/mol]:	446.58
CAS:	2519-10-0

Physical Properties

Property code	Value	Unit	Source
gf	863.82	kJ/mol	Joback Method
hf	547.08	kJ/mol	Joback Method
hfus	51.43	kJ/mol	Joback Method
hvap	108.37	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	9.006		Crippen Method
mcvol	365.750	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
tb	1167.12	K	Joback Method
tc	1462.29	K	Joback Method
tf	678.81	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1201.32	J/molxK	1167.12	Joback Method
cpg	1216.52	J/molxK	1216.31	Joback Method
cpg	1231.17	J/molxK	1265.51	Joback Method
cpg	1245.61	J/molxK	1314.70	Joback Method
cpg	1260.18	J/molxK	1363.90	Joback Method
cpg	1275.23	J/molxK	1413.09	Joback Method
cpg	1291.10	J/molxK	1462.29	Joback Method
dvisc	0.0002368	Paxs	678.81	Joback Method
dvisc	0.0001410	Paxs	760.20	Joback Method

dvisc	0.0000928	Paxs	841.58	Joback Method
dvisc	0.0000658	Paxs	922.96	Joback Method
dvisc	0.0000493	Paxs	1004.35	Joback Method
dvisc	0.0000386	Paxs	1085.73	Joback Method
dvisc	0.0000312	Paxs	1167.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2519100&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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