

P-cresol, 2,2'-ethylidene bis(6-(1-methylcyclohexyl))-

Inchi:	InChI=1S/C30H42O2/c1-20-16-23(27(31)25(18-20)29(4)12-8-6-9-13-29)22(3)24-17-21(2
InchiKey:	HKDAMRHFSHOFJA-UHFFFAOYSA-N
Formula:	C30H42O2
SMILES:	<chem>Cc1cc(C(C)c2cc(C)cc(C3(C)CCCCC3)c2O)c(O)c(C2(C)CCCCC2)c1</chem>
Mol. weight [g/mol]:	434.65
CAS:	26292-70-6

Physical Properties

Property code	Value	Unit	Source
gf	114.26	kJ/mol	Joback Method
hf	-456.13	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	113.77	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.310		Crippen Method
mcvol	376.060	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
tb	1159.46	K	Joback Method
tc	1434.37	K	Joback Method
tf	801.78	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.34	J/molxK	1159.46	Joback Method
cpg	1547.93	J/molxK	1205.28	Joback Method
cpg	1603.21	J/molxK	1251.10	Joback Method
cpg	1663.85	J/molxK	1296.91	Joback Method
cpg	1730.52	J/molxK	1342.73	Joback Method
cpg	1803.91	J/molxK	1388.55	Joback Method
cpg	1884.70	J/molxK	1434.37	Joback Method

Sources

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=C26292706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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