

Tetra-p-tolythene

Inchi:	InChI=1S/C30H28/c1-21-5-13-25(14-6-21)29(26-15-7-22(2)8-16-26)30(27-17-9-23(3)10-
InchiKey:	KNBCWMJBIJTDTTC-UHFFFAOYSA-N
Formula:	C30H28
SMILES:	<chem>Cc1ccc(C(=C(c2ccc(C)cc2)c2ccc(C)cc2)c2ccc(C)cc2)cc1</chem>
Mol. weight [g/mol]:	388.54
CAS:	5831-43-6

Physical Properties

Property code	Value	Unit	Source
gf	675.96	kJ/mol	Joback Method
hf	335.35	kJ/mol	Joback Method
hfus	45.65	kJ/mol	Joback Method
hvap	94.24	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	7.928		Crippen Method
mcvol	334.220	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
tb	1016.36	K	Joback Method
tc	1283.08	K	Joback Method
tf	550.62	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.30	J/molxK	1016.36	Joback Method
cpg	1073.45	J/molxK	1060.81	Joback Method
cpg	1089.48	J/molxK	1105.27	Joback Method
cpg	1104.60	J/molxK	1149.72	Joback Method
cpg	1119.03	J/molxK	1194.17	Joback Method
cpg	1132.97	J/molxK	1238.63	Joback Method
cpg	1146.63	J/molxK	1283.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5831436&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
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
mccvol:	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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