

1,1,2,2-Tetra-p-tolyethane

Inchi:	InChI=1S/C30H30/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:	MXGDNKSKKJBMPZ-UHFFFAOYSA-N
Formula:	C30H30
SMILES:	<chem>Cc1ccc(C(c2ccc(C)cc2)C(c2ccc(C)cc2)c2ccc(C)cc2)cc1</chem>
Mol. weight [g/mol]:	390.56
CAS:	40673-57-2

Physical Properties

Property code	Value	Unit	Source
gf	607.96	kJ/mol	Joback Method
hf	227.15	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	7.884		Crippen Method
mcvol	338.520	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
tb	1011.56	K	Joback Method
tc	1272.42	K	Joback Method
tf	553.62	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.57	J/molxK	1011.56	Joback Method
cpg	1103.26	J/molxK	1055.04	Joback Method
cpg	1118.54	J/molxK	1098.51	Joback Method
cpg	1132.59	J/molxK	1141.99	Joback Method
cpg	1145.57	J/molxK	1185.46	Joback Method
cpg	1157.66	J/molxK	1228.94	Joback Method
cpg	1169.02	J/molxK	1272.42	Joback Method
dvisc	0.0003350	Paxs	553.62	Joback Method
dvisc	0.0001685	Paxs	629.94	Joback Method

dvisc	0.0000983	Paxs	706.27	Joback Method
dvisc	0.0000637	Paxs	782.59	Joback Method
dvisc	0.0000446	Paxs	858.91	Joback Method
dvisc	0.0000331	Paxs	935.24	Joback Method
dvisc	0.0000257	Paxs	1011.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C40673572&Units=SI

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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