

1,4,6-triphenyl-1-hexene

Inchi:	InChI=1S/C24H24/c1-4-11-21(12-5-1)15-10-18-24(23-16-8-3-9-17-23)20-19-22-13-6-2-7
InchiKey:	HIMUTGZJUUFFDGY-XNTDXEJSSA-N
Formula:	C24H24
SMILES:	<chem>C(=Cc1ccccc1)CC(CCc1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	312.45

Physical Properties

Property code	Value	Unit	Source
gf	566.21	kJ/mol	Joback Method
hf	282.84	kJ/mol	Joback Method
hfus	36.72	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.506		Crippen Method
mcvol	273.440	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2338.20		NIST Webbook
tb	832.28	K	Joback Method
tc	1081.71	K	Joback Method
tf	419.42	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.16	J/molxK	832.28	Joback Method
cpg	885.20	J/molxK	1040.14	Joback Method
cpg	871.40	J/molxK	998.57	Joback Method
cpg	856.67	J/molxK	956.99	Joback Method
cpg	840.84	J/molxK	915.42	Joback Method
cpg	823.72	J/molxK	873.85	Joback Method
cpg	898.23	J/molxK	1081.71	Joback Method
dvisc	0.0000492	Paxs	832.28	Joback Method
dvisc	0.0000658	Paxs	763.47	Joback Method

dvisc	0.0000932	Paxs	694.66	Joback Method
dvisc	0.0001425	Paxs	625.85	Joback Method
dvisc	0.0002421	Paxs	557.04	Joback Method
dvisc	0.0004775	Paxs	488.23	Joback Method
dvisc	0.0011770	Paxs	419.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316217&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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