

2,4,6-triphenyl-1-heptene

Inchi:	InChI=1S/C25H26/c1-20(22-12-6-3-7-13-22)18-25(24-16-10-5-11-17-24)19-21(2)23-14-8
InchiKey:	BWOXCYYQUFTNFC-UHFFFAOYSA-N
Formula:	C25H26
SMILES:	<chem>C=C(CC(CC(C)c1ccccc1)c1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	571.26	kJ/mol	Joback Method
hf	255.34	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	7.067		Crippen Method
mcvol	287.530	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinsol	2360.00		NIST Webbook
tb	847.12	K	Joback Method
tc	1095.65	K	Joback Method
tf	405.05	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.90	J/mol×K	847.12	Joback Method
cpg	881.88	J/mol×K	888.54	Joback Method
cpg	899.33	J/mol×K	929.96	Joback Method
cpg	915.42	J/mol×K	971.38	Joback Method
cpg	930.30	J/mol×K	1012.81	Joback Method
cpg	944.14	J/mol×K	1054.23	Joback Method
cpg	957.10	J/mol×K	1095.65	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=R316306&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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