

all-trans-1,6-Diphenyl-1,3,5-hexatriene

Inchi:	InChI=1S/C18H16/c1(5-11-17-13-7-3-8-14-17)2-6-12-18-15-9-4-10-16-18/h1-16H/b2-1+,
InchiKey:	BOBLSBAZCVBABY-WPWUJOAOSA-N
Formula:	C18H16
SMILES:	<chem>C(=CC=Cc1ccccc1)C=Cc1ccccc1</chem>
Mol. weight [g/mol]:	232.32
CAS:	17329-15-6

Physical Properties

Property code	Value	Unit	Source
gf	566.16	kJ/mol	Joback Method
hf	409.87	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	60.09	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.969		Crippen Method
mcvol	204.060	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	677.08	K	Joback Method
tc	927.41	K	Joback Method
tf	330.22	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.46	J/molxK	677.08	Joback Method
cpg	529.13	J/molxK	718.80	Joback Method
cpg	545.36	J/molxK	760.52	Joback Method
cpg	560.31	J/molxK	802.25	Joback Method
cpg	574.17	J/molxK	843.97	Joback Method
cpg	587.10	J/molxK	885.69	Joback Method
cpg	599.27	J/molxK	927.41	Joback Method
dvisc	0.0017597	Paxs	330.22	Joback Method
dvisc	0.0007135	Paxs	388.03	Joback Method

dvisc	0.0003656	Paxs	445.84	Joback Method
dvisc	0.0002184	Paxs	503.65	Joback Method
dvisc	0.0001451	Paxs	561.46	Joback Method
dvisc	0.0001040	Paxs	619.27	Joback Method
dvisc	0.0000789	Paxs	677.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C17329156&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

Latest version available from:

<https://www.cheméo.com/cid/69-765-7/all-trans-1-6-Diphenyl-1-3-5-hexatriene.pdf>

Generated by Cheméo on 2024-04-26 06:42:14.650312585 +0000 UTC m=+16402983.570889897.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.