

trans-1,4-diphenylcyclohexane

Inchi:	InChI=1S/C18H20/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1-10,17-18
InchiKey:	VULCFZQVCFIKNK-UHFFFAOYSA-N
Formula:	C18H20
SMILES:	<chem>c1ccc(C2CCC(c3ccccc3)CC2)cc1</chem>
Mol. weight [g/mol]:	236.35
CAS:	21072-42-4

Physical Properties

Property code	Value	Unit	Source
affp	804.10	kJ/mol	NIST Webbook
basg	771.70	kJ/mol	NIST Webbook
gf	342.24	kJ/mol	Joback Method
hf	92.19	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	60.33	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.128		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
tb	679.48	K	Joback Method
tc	940.78	K	Joback Method
tf	348.60	K	Joback Method
vc	0.759	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.40	J/mol×K	679.48	Joback Method
cpg	596.72	J/mol×K	723.03	Joback Method
cpg	618.03	J/mol×K	766.58	Joback Method
cpg	637.43	J/mol×K	810.13	Joback Method
cpg	655.04	J/mol×K	853.68	Joback Method
cpg	670.98	J/mol×K	897.23	Joback Method
cpg	685.37	J/mol×K	940.78	Joback Method

dvisc	0.0023996	Paxs	348.60	Joback Method
dvisc	0.0011182	Paxs	403.75	Joback Method
dvisc	0.0006261	Paxs	458.89	Joback Method
dvisc	0.0003970	Paxs	514.04	Joback Method
dvisc	0.0002749	Paxs	569.19	Joback Method
dvisc	0.0002032	Paxs	624.33	Joback Method
dvisc	0.0001577	Paxs	679.48	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=C21072424&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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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