1,5-DIPHENYLBICYCLO[3.2.0]HEPTANE

Inchi: InChI=1S/C19H20/c1-3-8-16(9-4-1)18-12-7-13-19(18,15-14-18)17-10-5-2-6-11-17/h1-6,8
InchiKey: ITJCELKBMFHZCC-UHFFFAOYSA-N
Formula: C19H20
SMILES: c1ccc(C23CCCC2(c2ccccc2)CC3)cc1
Mol. weight [g/mol]: 248.37

Physical Properties

Property code	Value	Unit	Source
hf	215.00	kJ/mol	NIST Webbook
hfus	14.62	kJ/mol	Joback Method
ie	8.15	eV	Cheméo Relay (1.0)
logp	4.840		Crippen Method
mcvol	209.330	ml/mol	McGowan Method
tb	619.03	K	Cheméo Relay (1.0)
tf	451.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.06	J/mol×K	705.71	Joback Method
cpg	619.18	J/mol×K	751.79	Joback Method
cpg	640.42	J/mol×K	797.86	Joback Method
cpg	661.38	J/mol×K	843.94	Joback Method
cpg	682.68	J/mol×K	890.01	Joback Method
cpg	704.91	J/mol×K	936.09	Joback Method
cpg	728.68	J/mol×K	982.17	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94383672&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point