cis-1,2-Diphenyl-1-methylcyclopropane

Inchi: InChI=1S/C16H16/c1-16(14-10-6-3-7-11-14)12-15(16)13-8-4-2-5-9-13/h2-11,15H,12H2,1
InchiKey: MEPKNRHJYLWJON-JKSUJKDBSA-N
Formula: C16H16
SMILES: CC1(c2ccccc2)CC1c1ccccc1
Mol. weight [g/mol]: 208.30
CAS: 14161-72-9

Physical Properties

Property code	Value	Unit	Source
gf	356.21	kJ/mol	Joback Method
hf	167.19	kJ/mol	Joback Method
hfus	18.19	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Joback Method
ie	7.90 ± 0.03	eV	NIST Webbook
log10ws	-4.26		Crippen Method
logp	4.132		Crippen Method
mcvol	177.920	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	621.15	K	Joback Method
tc	878.60	K	Joback Method
tf	360.52	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.16	J/mol×K	621.15	Joback Method
cpg	476.92	J/mol×K	664.06	Joback Method
cpg	495.16	J/mol×K	706.97	Joback Method
cpg	512.16	J/mol×K	749.87	Joback Method
cpg	528.21	J/mol×K	792.78	Joback Method
cpg	543.60	J/mol×K	835.69	Joback Method
cpg	558.60	J/mol×K	878.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14161729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
ie:	Ionization energy
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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