(trans)-1,1'-(1,2-cyclopropanediyl)bisbenzene

Other names: trans-1,2-Diphenylcyclopropane
Inchi: InChI=1S/C15H14/c1-3-7-12(8-4-1)14-11-15(14)13-9-5-2-6-10-13/h1-10,14-15H,11H2/t1
InchiKey: ZSIYTDQNAOYUNE-HUUCEWRRSA-N
Formula: C15H14
SMILES: c1ccc(C2CC2c2ccccc2)cc1
Mol. weight [g/mol]: 194.27
CAS: 1138-47-2

Physical Properties

Property code	Value	Unit	Source
chl	-8070.00 ± 3.00	kJ/mol	NIST Webbook
gf	353.28	kJ/mol	Joback Method
hf	172.59	kJ/mol	Joback Method
hfl	166.00 ± 3.00	kJ/mol	NIST Webbook
hfus	21.89	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
ie	8.05	eV	NIST Webbook
log10ws	-4.13		Crippen Method
logp	3.958		Crippen Method
mcvol	163.830	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	598.03	K	Joback Method
tc	850.80	K	Joback Method
tf	325.35	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.95	J/mol×K	598.03	Joback Method
cpg	428.59	J/mol×K	640.16	Joback Method
cpg	446.57	J/mol×K	682.29	Joback Method
cpg	463.05	J/mol×K	724.42	Joback Method
cpg	478.14	J/mol×K	766.55	Joback Method

cpg	491.97	J/mol×K	808.67	Joback Method
cpg	504.67	J/mol×K	850.80	Joback Method
dvisc	0.0018909	Pa×s	325.35	Joback Method
dvisc	0.0012846	Pa×s	370.80	Joback Method
dvisc	0.0009496	Pa×s	416.24	Joback Method
dvisc	0.0007450	Pa×s	461.69	Joback Method
dvisc	0.0006105	Pa×s	507.14	Joback Method
dvisc	0.0005169	Pa×s	552.58	Joback Method
dvisc	0.0004488	Pa×s	598.03	Joback Method

Sources

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=C1138472&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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