1(Hydroxymethyl)-2,2-diphenylcyclopropane

Inchi: InChI=1S/C16H16O/c17-12-15-11-16(15,13-7-3-1-4-8-13)14-9-5-2-6-10-14/h1-10,15,17H
InchiKey: DKKWWWHVSKHVQJ-UHFFFAOYSA-N
Formula: C16H16O
SMILES: OCC1CC1(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	219.39	kJ/mol	Joback Method
hf	14.96	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.985		Crippen Method
mcvol	183.790	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	713.33	K	Joback Method
tc	947.25	K	Joback Method
tf	421.34	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.37	J/mol×K	713.33	Joback Method
cpg	530.92	J/mol×K	752.32	Joback Method
cpg	545.67	J/mol×K	791.30	Joback Method
cpg	559.85	J/mol×K	830.29	Joback Method
cpg	573.66	J/mol×K	869.28	Joback Method
cpg	587.32	J/mol×K	908.27	Joback Method
cpg	601.06	J/mol×K	947.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000909&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
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