

cis-Hydroxymethylcyclopropane, 2-methyl-2-phenyl

Inchi: InChI=1S/C11H14O/c1-11(7-10(11)8-12)9-5-3-2-4-6-9/h2-6,10,12H,7-8H2,1H3/t10-,11+/m1
InchiKey: UHQXBASRPLGYEL-MNOVXSKEA-N
Formula: C11H14O
SMILES: CC1(c2ccccc2)CC1CO
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	64.88	kJ/mol	Joback Method
hf	-118.37	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	57.49	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.956		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1295.00		NIST Webbook
tb	572.25	K	Joback Method
tc	783.32	K	Joback Method
tf	338.57	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.20	J/mol×K	572.25	Joback Method
cpg	358.07	J/mol×K	607.43	Joback Method
cpg	371.00	J/mol×K	642.61	Joback Method
cpg	383.13	J/mol×K	677.78	Joback Method
cpg	394.59	J/mol×K	712.96	Joback Method
cpg	405.53	J/mol×K	748.14	Joback Method
cpg	416.09	J/mol×K	783.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13535&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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