

Cyclopropanemethanol, 1-phenyl-

Other names:	1-Phenyl cyclopropane-1-methanol «alpha»-Cyclopropylbenzyl alcohol (1-Phenylcyclopropyl)methanol 1-phenylcyclopropanemethanol
Inchi:	InChI=1S/C10H12O/c11-8-10(6-7-10)9-4-2-1-3-5-9/h1-5,11H,6-8H2
InchiKey:	APALRPYIDIBHQN-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	OCC1(c2ccccc2)CC1
Mol. weight [g/mol]:	148.20
CAS:	31729-66-5

Physical Properties

Property code	Value	Unit	Source
gf	64.17	kJ/mol	Joback Method
hf	-77.39	kJ/mol	Joback Method
hfus	11.62	kJ/mol	Joback Method
hvap	55.57	kJ/mol	Joback Method
ie	8.35	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.710		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	554.04	K	Joback Method
tc	768.75	K	Joback Method
tf	331.54	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.08	J/mol×K	554.04	Joback Method
cpg	308.81	J/mol×K	589.82	Joback Method
cpg	320.56	J/mol×K	625.61	Joback Method
cpg	331.50	J/mol×K	661.39	Joback Method

cpg	341.76	J/mol×K	697.18	Joback Method
cpg	351.50	J/mol×K	732.96	Joback Method
cpg	360.86	J/mol×K	768.75	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=C31729665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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