

trans-Hydroxymethylcyclopropane, 2-methyl-2-phenyl

Inchi:	InChI=1S/C10H12O/c11-7-9-6-10(9)8-4-2-1-3-5-8/h1-5,9-11H,6-7H2/t9-,10-/m0/s1
InchiKey:	CEZOORGGKZLLAO-UWVGGRQHSA-N
Formula:	C10H12O
SMILES:	OCC1CC1c1ccccc1
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
gf	61.95	kJ/mol	Joback Method
hf	-112.97	kJ/mol	Joback Method
hfus	18.99	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.782		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinsol	1340.00		NIST Webbook
tb	549.13	K	Joback Method
tc	755.41	K	Joback Method
tf	303.40	K	Joback Method
vc	0.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.63	J/molxK	549.13	Joback Method
cpg	312.17	J/molxK	583.51	Joback Method
cpg	324.83	J/molxK	617.89	Joback Method
cpg	336.67	J/molxK	652.27	Joback Method
cpg	347.73	J/molxK	686.65	Joback Method
cpg	358.07	J/molxK	721.03	Joback Method
cpg	367.74	J/molxK	755.41	Joback Method
dvisc	0.0069752	Paxs	303.40	Joback Method
dvisc	0.0028970	Paxs	344.35	Joback Method

dvisc	0.0014503	Paxs	385.31	Joback Method
dvisc	0.0008293	Paxs	426.26	Joback Method
dvisc	0.0005230	Paxs	467.22	Joback Method
dvisc	0.0003553	Paxs	508.18	Joback Method
dvisc	0.0002557	Paxs	549.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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