

2,2,4,4-Tetramethylcyclobutane-1,3-diol, cis

Inchi:	InChI=1S/C8H16O2/c1-7(2)5(9)8(3,4)6(7)10/h5-6,9-10H,1-4H3/t5-,6+
InchiKey:	FQXGHZNSUOHCLO-OLQVQODUSA-N
Formula:	C8H16O2
SMILES:	CC1(C)C(O)C(C)(C)C1O
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	-242.62	kJ/mol	Joback Method
hf	-476.81	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	63.62	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	0.774		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinsol	1069.00		NIST Webbook
tb	564.28	K	Joback Method
tc	745.68	K	Joback Method
tf	351.06	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.40	J/mol×K	564.28	Joback Method
cpg	344.79	J/mol×K	594.51	Joback Method
cpg	355.58	J/mol×K	624.75	Joback Method
cpg	365.89	J/mol×K	654.98	Joback Method
cpg	375.84	J/mol×K	685.21	Joback Method
cpg	385.53	J/mol×K	715.45	Joback Method
cpg	395.09	J/mol×K	745.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R81314&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
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
mccvol:	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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