

1,3-DIHYDRO-1-HYDROXY-3,3-DIMETHYL-1(M-TO

Inchi:	InChI=1S/C17H18O2/c1-12-7-6-8-13(11-12)17(18)15-10-5-4-9-14(15)16(2,3)19-17/h4-11
InchiKey:	XMLTURDDADEPER-UHFFFAOYSA-N
Formula:	C17H18O2
SMILES:	Cc1cccc(C2(O)OC(C)(C)c3ccccc32)c1
Mol. weight [g/mol]:	254.33

Physical Properties

Property code	Value	Unit	Source
hfus	25.77	kJ/mol	Joback Method
logp	3.454		Crippen Method
mcpvol	203.750	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.61	J/mol×K	773.36	Joback Method
cpg	608.85	J/mol×K	812.70	Joback Method
cpg	625.15	J/mol×K	852.05	Joback Method
cpg	641.84	J/mol×K	891.39	Joback Method
cpg	659.23	J/mol×K	930.74	Joback Method
cpg	677.63	J/mol×K	970.08	Joback Method
cpg	697.35	J/mol×K	1009.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7002473&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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