

1-HYDROXY-P-MENTH-3-ONE

Inchi:	InChI=1S/C10H18O2/c1-7(2)8-4-5-10(3,12)6-9(8)11/h7-8,12H,4-6H2,1-3H3
InchiKey:	MITMEWYOGQSHSC-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)C1CCC(C)(O)CC1=O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
hfus	8.34	kJ/mol	Joback Method
ie	9.27	eV	Cheméo Relay (1.0)
log10ws	-1.00		Cheméo Relay (1.0)
logp	1.763		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
tb	505.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.08	J/mol×K	602.88	Joback Method
cpg	418.34	J/mol×K	637.96	Joback Method
cpg	433.79	J/mol×K	673.03	Joback Method
cpg	448.52	J/mol×K	708.11	Joback Method
cpg	462.59	J/mol×K	743.19	Joback Method
cpg	476.08	J/mol×K	778.27	Joback Method
cpg	489.06	J/mol×K	813.34	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=C63865645&Units=SI>

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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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