

5-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one

Other names:	5-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one 2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl 5-ethyl-2-hydroxy-3-methylcyclopent-2-en-1-one
Inchi:	InChI=1S/C8H12O2/c1-3-6-4-5(2)7(9)8(6)10/h6,9H,3-4H2,1-2H3
InchiKey:	ARHWUYVUNJLMRR-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CCC1CC(C)=C(O)C1=O
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
hfus	14.45	kJ/mol	Joback Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
rinpol	1135.00		NIST Webbook
ripol	1799.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.61	J/mol×K	566.84	Joback Method
cpg	295.46	J/mol×K	600.51	Joback Method
cpg	306.81	J/mol×K	634.19	Joback Method
cpg	317.65	J/mol×K	667.86	Joback Method
cpg	327.96	J/mol×K	701.53	Joback Method
cpg	337.75	J/mol×K	735.21	Joback Method
cpg	347.01	J/mol×K	768.88	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
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=C53263584&Units=SI>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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