3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE

Other names:	3-Ethyl-2-hydroxy-2-cyclopenten-1-one
	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl
	2-Hydroxy-3-ethyl-2-cyclopenten-1-one
	3-Ethyl-2-hydroxy-2-cyclopentenone
	3-ethyl-2-hydroxycyclopent-2-en-1-one
Inchi:	InChI=1S/C7H10O2/c1-2-5-3-4-6(8)7(5)9/h9H,2-4H2,1H3
InchiKey:	JHWFWLUAUPZUCP-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CCC1=C(O)C(=O)CC1
Mol. weight [g/mol]:	126.15

Physical Properties

Property code	Value	Unit	Source
hfus	10.79	kJ/mol	Joback Method
logp	1.571		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
rinpol	1100.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1891.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.75	J/mol×K	548.63	Joback Method
cpg	247.22	J/mol×K	582.83	Joback Method
cpg	257.24	J/mol×K	617.04	Joback Method
cpg	266.79	J/mol×K	651.24	Joback Method
cpg	275.88	J/mol×K	685.45	Joback Method
cpg	284.51	J/mol×K	719.65	Joback Method
cpg	292.68	J/mol×K	753.86	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=C21835018&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

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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