4-Ethyl-2-hydroxycyclopent-2-en-1-one

Other names: 4-Ethyl-2-hydroxy-2-cyclopenten-1-one
Inchi: InChI=1S/C7H10O2/c1-2-5-3-6(8)7(9)4-5/h3,5,8H,2,4H2,1H3
InchiKey: CVBNEZQOINGLSS-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CCC1C=C(O)C(=O)C1
Mol. weight [g/mol]: 126.15
CAS: 28017-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-194.47	kJ/mol	Joback Method
hf	-370.95	kJ/mol	Joback Method
hfus	12.25	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
tb	538.98	K	Joback Method
tc	742.99	K	Joback Method
tf	321.87	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.25	J/mol×K	538.98	Joback Method
cpg	250.36	J/mol×K	572.98	Joback Method
cpg	260.98	J/mol×K	606.98	Joback Method
cpg	271.11	J/mol×K	640.98	Joback Method
cpg	280.75	J/mol×K	674.99	Joback Method
cpg	289.88	J/mol×K	708.99	Joback Method

cpg	298.51	J/mol×K	742.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28017621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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