

4-Hydroxy-cryptone

Other names:	4-hydroxy-crypton
Inchi:	InChI=1S/C9H14O2/c1-7(2)9(11)5-3-8(10)4-6-9/h3,5,7,11H,4,6H2,1-2H3
InchiKey:	CONYQDCNFROMMQ-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC(C)C1(O)C=CC(=O)CC1
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
gf	-188.03	kJ/mol	Joback Method
hf	-396.96	kJ/mol	Joback Method
hfus	5.90	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.293		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2269.00		NIST Webbook
tb	583.83	K	Joback Method
tc	799.88	K	Joback Method
tf	337.27	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.02	J/molxK	583.83	Joback Method
cpg	345.00	J/molxK	619.84	Joback Method
cpg	358.22	J/molxK	655.85	Joback Method
cpg	370.78	J/molxK	691.85	Joback Method
cpg	382.75	J/molxK	727.86	Joback Method

cpg	394.22	J/mol×K	763.87	Joback Method
cpg	405.27	J/mol×K	799.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R440434&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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