

2-Hydroxypinan-3-one

Other names:	2-hydroxy-2,6,6-trimethylbicyclo[3.1.1]heptan-3-one
Inchi:	InChI=1S/C10H16O2/c1-9(2)6-4-7(9)10(3,12)8(11)5-6/h6-7,12H,4-5H2,1-3H3
InchiKey:	VZRRCQOUNSHSGB-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC1(O)C(=O)CC2CC1C2(C)C
Mol. weight [g/mol]:	168.23
CAS:	10136-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-143.09	kJ/mol	Joback Method
hf	-410.42	kJ/mol	Joback Method
hfus	8.97	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.373		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1255.80		NIST Webbook
rinpol	1255.80		NIST Webbook
ripol	1983.00		NIST Webbook
tb	597.09	K	Joback Method
tc	811.66	K	Joback Method
tf	403.18	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.29	J/mol×K	597.09	Joback Method
cpg	399.17	J/mol×K	632.85	Joback Method
cpg	413.28	J/mol×K	668.61	Joback Method

cpg	426.81	J/mol×K	704.38	Joback Method
cpg	439.96	J/mol×K	740.14	Joback Method
cpg	452.93	J/mol×K	775.90	Joback Method
cpg	465.91	J/mol×K	811.66	Joback Method

Sources

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=C10136659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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