2-hydroxyisopiperitone

Inchi: InChI=1S/C10H16O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h7-9,11H,1,4-5H2,2-3H3
InchiKey: CIPUCJXOPVIIPN-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: C=C(C)C1CCC(C)C(O)C1=O
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-137.77	kJ/mol	Joback Method
hf	-410.38	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.539		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
tb	594.97	K	Joback Method
tc	801.08	K	Joback Method
tf	314.68	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	594.97	Joback Method
cpg	400.36	J/mol×K	629.32	Joback Method
cpg	415.79	J/mol×K	663.67	Joback Method
cpg	430.40	J/mol×K	698.02	Joback Method
cpg	444.19	J/mol×K	732.37	Joback Method
cpg	457.14	J/mol×K	766.73	Joback Method
cpg	469.25	J/mol×K	801.08	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=R226154&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume