4-oxo- «beta»-cyclocitral

Inchi: InChI=1S/C9H12O2/c1-9(2)4-3-8(11)5-7(9)6-10/h5-6H,3-4H2,1-2H3
InchiKey: AODZASMSAIPDLQ-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CC1(C)CCC(=O)C=C1C=O
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
gf	-157.92	kJ/mol	Joback Method
hf	-336.50	kJ/mol	Joback Method
hfus	7.24	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.501		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
ripol	1951.00		NIST Webbook
ripol	1951.00		NIST Webbook
tb	545.73	K	Joback Method
tc	779.26	K	Joback Method
tf	345.97	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.40	J/mol×K	545.73	Joback Method
cpg	309.96	J/mol×K	584.65	Joback Method
cpg	323.66	J/mol×K	623.57	Joback Method
cpg	336.62	J/mol×K	662.49	Joback Method
cpg	348.92	J/mol×K	701.41	Joback Method
cpg	360.66	J/mol×K	740.34	Joback Method
cpg	371.94	J/mol×K	779.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R344128&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume