2-Cyclopenten-1-one, 3-(1-methylethyl)-

Inchi: InChI=1S/C8H12O/c1-6(2)7-3-4-8(9)5-7/h5-6H,3-4H2,1-2H3
InchiKey: OGHGFNURIXNXEM-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC(C)C1=CC(=O)CC1
Mol. weight [g/mol]: 124.18
CAS: 1619-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-43.96	kJ/mol	Joback Method
hf	-224.30	kJ/mol	Joback Method
hfus	6.16	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1070.00		NIST Webbook
tb	473.91	K	Joback Method
tc	694.76	K	Joback Method
tf	261.56	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.69	J/mol×K	473.91	Joback Method
cpg	245.95	J/mol×K	510.72	Joback Method
cpg	259.54	J/mol×K	547.53	Joback Method
cpg	272.47	J/mol×K	584.34	Joback Method
cpg	284.74	J/mol×K	621.15	Joback Method
cpg	296.36	J/mol×K	657.95	Joback Method
cpg	307.33	J/mol×K	694.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1619289&Units=SI
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

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