2-Acetonylcyclohexanone

Inchi: InChI=1S/C9H14O2/c1-7(10)6-8-4-2-3-5-9(8)11/h8H,2-6H2,1H3
InchiKey: ZBEKDHUCMTXKAO-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC(=O)CC1CCCCC1=O
Mol. weight [g/mol]: 154.21
CAS: 6126-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-202.16	kJ/mol	Joback Method
hf	-425.05	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.725		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	546.56	K	Joback Method
tc	772.73	K	Joback Method
tf	316.72	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.16	J/mol×K	546.56	Joback Method
cpg	331.03	J/mol×K	584.25	Joback Method
cpg	347.01	J/mol×K	621.95	Joback Method
cpg	362.09	J/mol×K	659.64	Joback Method
cpg	376.28	J/mol×K	697.34	Joback Method
cpg	389.55	J/mol×K	735.03	Joback Method
cpg	401.92	J/mol×K	772.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6126530&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