4-Isopropenylcyclohexanone

Inchi: InChI=1S/C9H14O/c1-7(2)8-3-5-9(10)6-4-8/h8H,1,3-6H2,2H3
InchiKey: YQMUZRNPCVSBEH-UHFFFAOYSA-N
Formula: C9H14O
SMILES: C=C(C)C1CCC(=O)CC1
Mol. weight [g/mol]: 138.21
CAS: 22460-53-3

Physical Properties

Property code	Value	Unit	Source
gf	6.05	kJ/mol	Joback Method
hf	-196.83	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1161.00		NIST Webbook
tb	489.25	K	Joback Method
tc	715.56	K	Joback Method
tf	251.07	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.45	J/mol×K	489.25	Joback Method
cpg	291.11	J/mol×K	526.97	Joback Method
cpg	307.89	J/mol×K	564.69	Joback Method
cpg	323.80	J/mol×K	602.41	Joback Method
cpg	338.83	J/mol×K	640.13	Joback Method
cpg	352.99	J/mol×K	677.84	Joback Method

cpg	366.29	J/mol×K	715.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22460533&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