4-acetylmethylcyclohexene

Inchi: InChI=1S/C9H14O/c1-8(10)7-9-5-3-2-4-6-9/h2-3,9H,4-7H2,1H3
InchiKey: MVIWJWRXINGWNY-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC(=O)CC1CC=CCC1
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-49.61	kJ/mol	Joback Method
hf	-229.57	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1141.00		NIST Webbook
tb	477.90	K	Joback Method
tc	690.34	K	Joback Method
tf	249.26	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.16	J/mol×K	477.90	Joback Method
cpg	338.88	J/mol×K	654.93	Joback Method
cpg	326.03	J/mol×K	619.53	Joback Method
cpg	312.37	J/mol×K	584.12	Joback Method
cpg	297.85	J/mol×K	548.71	Joback Method
cpg	282.46	J/mol×K	513.31	Joback Method
cpg	350.92	J/mol×K	690.34	Joback Method
dvisc	0.0003064	Pa×s	477.90	Joback Method

dvisc	0.0003973	Pa×s	439.79	Joback Method
dvisc	0.0005411	Pa×s	401.69	Joback Method
dvisc	0.0007864	Pa×s	363.58	Joback Method
dvisc	0.0012474	Pa×s	325.47	Joback Method
dvisc	0.0022361	Pa×s	287.37	Joback Method
dvisc	0.0047916	Pa×s	249.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R512524&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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