2-Cyclohexen-1-one, 4,5-dimethyl-

Other names: 4,5-Dimethylcyclohexen-2-one
4,5-Dimethyl-2-cyclohexen-1-one
Inchi: InChI=1S/C8H12O/c1-6-3-4-8(9)5-7(6)2/h3-4,6-7H,5H2,1-2H3
InchiKey: XADBPCVQACZOEL-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1C=CC(=O)CC1C
Mol. weight [g/mol]: 124.18
CAS: 5715-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-59.41	kJ/mol	Joback Method
hf	-254.39	kJ/mol	Joback Method
hfus	10.11	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.788		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1016.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	464.30	K	Joback Method
tc	686.73	K	Joback Method
tf	252.04	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.85	J/mol×K	464.30	Joback Method
cpg	247.81	J/mol×K	501.37	Joback Method
cpg	263.10	J/mol×K	538.44	Joback Method
cpg	277.71	J/mol×K	575.51	Joback Method
cpg	291.61	J/mol×K	612.58	Joback Method

cpg	304.79	J/mol×K	649.66	Joback Method
cpg	317.25	J/mol×K	686.73	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=C5715253&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume