Phorone

Other names:	2,5-Heptadien-4-one, 2,6-dimethyl-
	s-Diisopropylidene acetone
	Diisobutenyl ketone
	Diisopropylidene acetone
	Foron
	sym-Diisopropylidene acetone
	Phoron
	2,6-Dimethyl-2,5-heptadien-4-one
	NSC 38718
	2,6-dimethylhepta-2,5-dien-4-one
Inchi:	InChI=1S/C9H14O/c1-7(2)5-9(10)6-8(3)4/h5-6H,1-4H3
InchiKey:	MTZWHHIREPJPTG-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(C)=CC(=O)C=C(C)C
Mol. weight [g/mol]:	138.21
CAS:	504-20-1

Physical Properties

Property code	Value	Unit	Source
gf	39.32	kJ/mol	Joback Method
hf	-126.81	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.488		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1092.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	470.70	K	NIST Webbook
tb	470.15 ± 2.00	K	NIST Webbook
tc	665.67	K	Joback Method
tf	299.00 ± 0.50	K	NIST Webbook
tf	301.15 ± 2.00	K	NIST Webbook
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.84	J/mol×K	467.27	Joback Method
cpg	278.12	J/mol×K	500.34	Joback Method
cpg	290.66	J/mol×K	533.40	Joback Method
cpg	302.48	J/mol×K	566.47	Joback Method
cpg	313.64	J/mol×K	599.54	Joback Method
cpg	324.18	J/mol×K	632.60	Joback Method
cpg	334.13	J/mol×K	665.67	Joback Method
hvapt	54.10	kJ/mol	393.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C504201&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
hvapt: Enthalpy of vaporization at a given temperature
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