2,4,4-trimethylcyclohexanone

Inchi: InChI=1S/C9H16O/c1-7-6-9(2,3)5-4-8(7)10/h7H,4-6H2,1-3H3
InchiKey: JEANOXXXGPLTOI-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1CC(C)(C)CCC1=O
Mol. weight [g/mol]: 140.22
CAS: 2230-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-86.44	kJ/mol	Joback Method
hf	-317.57	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	38.84	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	464.00 ± 3.00	K	NIST Webbook
tc	714.57	K	Joback Method
tf	286.45	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.44	J/mol×K	488.26	Joback Method
cpg	310.90	J/mol×K	525.98	Joback Method
cpg	328.31	J/mol×K	563.70	Joback Method
cpg	344.77	J/mol×K	601.42	Joback Method
cpg	360.36	J/mol×K	639.14	Joback Method
cpg	375.16	J/mol×K	676.85	Joback Method
cpg	389.26	J/mol×K	714.57	Joback Method

Sources

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=C2230708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume