Cyclohexanone, 2-isopropyl-2,5-dimethyl-

Other names: 2-Isopropyl-2,5-dimethyl-cyclohexanone
Inchi: InChI=1S/C11H20O/c1-8(2)11(4)6-5-9(3)7-10(11)12/h8-9H,5-7H2,1-4H3
InchiKey: PFXHRFGMSHIJQV-UHFFFAOYSA-N
Formula: C11H20O
SMILES: CC1CCC(C)(C(C)C)C(=O)C1
Mol. weight [g/mol]: 168.28
CAS: 20144-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-72.04	kJ/mol	Joback Method
hf	-364.13	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	42.91	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	3.038		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
tb	533.58	K	Joback Method
tc	757.23	K	Joback Method
tf	293.99	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.18	J/mol×K	533.58	Joback Method
cpg	407.69	J/mol×K	570.85	Joback Method
cpg	427.08	J/mol×K	608.13	Joback Method
cpg	445.43	J/mol×K	645.40	Joback Method
cpg	462.85	J/mol×K	682.68	Joback Method
cpg	479.41	J/mol×K	719.95	Joback Method

cpg	495.21	J/mol×K	757.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20144449&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
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