Cyclohexanone, sec.-butyl, # 1

Other names:	Cyclohexanone, sec.-butyl, # 2
	Cyclohexanone, sec-butyl, # 2
	Cyclohexanone, sec-butyl, # 1
	2-sec-butylcyclohexan-1-one
Inchi:	InChI=1S/C10H18O/c1-3-8(2)9-6-4-5-7-10(9)11/h8-9H,3-7H2,1-2H3
InchiKey:	RQXTZKGDMNIWJF-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CCC(C)C1CCCCC1=O
Mol. weight [g/mol]:	154.25
CAS:	14765-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-67.26	kJ/mol	Joback Method
hf	-338.39	kJ/mol	Joback Method
hfus	9.48	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	515.13	K	Joback Method
tc	733.50	K	Joback Method
tf	263.06	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.43	J/mol×K	515.13	Joback Method
cpg	357.81	J/mol×K	551.52	Joback Method
cpg	376.25	J/mol×K	587.92	Joback Method
cpg	393.75	J/mol×K	624.31	Joback Method
cpg	410.32	J/mol×K	660.71	Joback Method
cpg	425.96	J/mol×K	697.10	Joback Method
cpg	440.66	J/mol×K	733.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14765301&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume