2-Methyl-4-(1-methylethyl)-2-cyclohexenone

Inchi: InChI=1S/C10H16O/c1-7(2)9-4-5-10(11)8(3)6-9/h6-7,9H,4-5H2,1-3H3
InchiKey: BPIZZOZTEBWEPT-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CC(C(C)C)CCC1=O
Mol. weight [g/mol]: 152.23
CAS: 41469-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.93	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	519.27	K	Joback Method
tc	741.04	K	Joback Method
tf	276.34	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.40	J/mol×K	519.27	Joback Method
cpg	339.21	J/mol×K	556.23	Joback Method
cpg	356.17	J/mol×K	593.19	Joback Method
cpg	372.28	J/mol×K	630.16	Joback Method
cpg	387.53	J/mol×K	667.12	Joback Method
cpg	401.93	J/mol×K	704.08	Joback Method
cpg	415.47	J/mol×K	741.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41469469&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