2-Cyclohexen-1-one, 2-hydroxy-6-methyl-3-(1-methylethyl)-

Other names: 2-hydroxy-3-(isopropyl)-6-methylcyclohex-2-en-1-one
2-Hydroxy-3-isopropyl-6-methylcyclohex-2-enone
Inchi: InChI=1S/C10H16O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h6-7,12H,4-5H2,1-3H3
InchiKey: POVACFJTDXZOQT-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC(C)C1=C(O)C(=O)C(C)CC1
Mol. weight [g/mol]: 168.23
CAS: 54783-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-193.38	kJ/mol	Joback Method
hf	-455.78	kJ/mol	Joback Method
hfus	14.01	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.454		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1274.10		NIST Webbook
rinpol	1274.10		NIST Webbook
tb	616.43	K	Joback Method
tc	823.06	K	Joback Method
tf	349.68	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.65	J/mol×K	616.43	Joback Method
cpg	395.28	J/mol×K	650.87	Joback Method
cpg	409.19	J/mol×K	685.31	Joback Method
cpg	422.36	J/mol×K	719.75	Joback Method
cpg	434.79	J/mol×K	754.19	Joback Method

cpg	446.47	J/mol×K	788.62	Joback Method
cpg	457.40	J/mol×K	823.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54783367&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