2-Cyclohexen-1-one, 4-hydroxy-3-methyl-6-(1-methylethyl)-, trans-

Other names: 4-Hydroxy-6-isopropyl-3-methylcyclohex-2-enone
Inchi: InChI=1S/C10H16O2/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4,6,8-9,11H,5H2,1-3H3/t8-,9+/m1/s
InchiKey: HEJGMQATUPGCRD-BDAKNGLRSA-N
Formula: C10H16O2
SMILES: CC1=CC(=O)C(C(C)C)CC1O
Mol. weight [g/mol]: 168.23
CAS: 55955-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-191.46	kJ/mol	Joback Method
hf	-464.65	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	59.47	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.539		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1432.30		NIST Webbook
rinpol	1432.30		NIST Webbook
tb	606.78	K	Joback Method
tc	812.40	K	Joback Method
tf	332.92	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.06	J/mol×K	606.78	Joback Method
cpg	398.33	J/mol×K	641.05	Joback Method
cpg	412.83	J/mol×K	675.32	Joback Method
cpg	426.57	J/mol×K	709.59	Joback Method
cpg	439.53	J/mol×K	743.86	Joback Method
cpg	451.71	J/mol×K	778.13	Joback Method

cpg	463.09	J/mol×K	812.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55955538&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

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

Latest version available from:
https://www.chemeo.com/cid/86-021-3/2-Cyclohexen-1-one-4-hydroxy-3-methyl-6-1-methylethyl-trans.pdf
Generated by Cheméo on 2025-12-05 22:08:15.937396705 +0000 UTC m=+4720693.467437360.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.