Cyclohexanol, 2-methyl-4-tert.-octyl, acetate

Other names: Cyclohexanol, 2-methyl-4-tert-octyl, acetate
Inchi: InChI=1S/C17H32O2/c1-12-10-14(8-9-15(12)19-13(2)18)17(6,7)11-16(3,4)5/h12,14-15H
InchiKey: VZVLBDDGOOHNPU-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CC(=O)OC1CCC(C(C)(C)CC(C)(C)C)CC1C
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-126.95	kJ/mol	Joback Method
hf	-642.87	kJ/mol	Joback Method
hfus	21.72	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.817		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	668.40	K	Joback Method
tc	875.03	K	Joback Method
tf	357.25	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.31	J/mol×K	668.40	Joback Method
cpg	837.88	J/mol×K	840.59	Joback Method
cpg	820.05	J/mol×K	806.15	Joback Method
cpg	800.93	J/mol×K	771.71	Joback Method
cpg	780.47	J/mol×K	737.28	Joback Method
cpg	758.62	J/mol×K	702.84	Joback Method

cpg	854.48	J/mol×K	875.03	Joback Method
dvisc	0.0001198	Pa×s	668.40	Joback Method
dvisc	0.0001618	Pa×s	616.54	Joback Method
dvisc	0.0002310	Pa×s	564.68	Joback Method
dvisc	0.0003544	Pa×s	512.83	Joback Method
dvisc	0.0005986	Pa×s	460.97	Joback Method
dvisc	0.0011548	Pa×s	409.11	Joback Method
dvisc	0.0026959	Pa×s	357.25	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R17739&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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