

4-tert-Butylcyclohexyl acetate

Other names:	Acetic acid p-tert-butylcyclohexyl ester Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate p-tert-Butyl cyclohexyl acetate Acetic acid, (4-tert-butylcyclohexyl) ester Cyclohexanol, 4-tert-butyl-, acetate Vertenex 4-tert-Butylcyclohexanol acetate 4-tert-Butylhexahydrophenyl acetate 4-t-Butylcyclohexyl acetate Cyclohexanol, 4-(1,1-dimethylethyl)-, 1-acetate NSC 163103
Inchi:	InChI=1S/C12H22O2/c1-9(13)14-11-7-5-10(6-8-11)12(2,3)4/h10-11H,5-8H2,1-4H3/t10?,
InchiKey:	MBZRJSQZCBXRGK-CACVWKRDSA-N
Formula:	C12H22O2
SMILES:	CC(=O)OC1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]:	198.30
CAS:	32210-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-164.18	kJ/mol	Joback Method
hf	-510.58	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.154		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1346.20		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1348.00		NIST Webbook

tb	561.90	K	Joback Method
tc	773.24	K	Joback Method
tf	302.72	K	Joback Method
vc	0.652	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.11	J/mol×K	561.90	Joback Method
cpg	478.84	J/mol×K	597.12	Joback Method
cpg	498.39	J/mol×K	632.35	Joback Method
cpg	516.77	J/mol×K	667.57	Joback Method
cpg	534.02	J/mol×K	702.79	Joback Method
cpg	550.18	J/mol×K	738.01	Joback Method
cpg	565.28	J/mol×K	773.24	Joback Method
dvisc	0.0039043	Pa×s	302.72	Joback Method
dvisc	0.0017642	Pa×s	345.92	Joback Method
dvisc	0.0009509	Pa×s	389.11	Joback Method
dvisc	0.0005799	Pa×s	432.31	Joback Method
dvisc	0.0003869	Pa×s	475.51	Joback Method
dvisc	0.0002762	Pa×s	518.70	Joback Method
dvisc	0.0002076	Pa×s	561.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32210234&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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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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