Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate, trans-

Other names: p-tert-Butyl cyclohexyl-acetate trans
4-tert-Butylcyclohexyl acetate, (E)-
trans-4-tert-butylcyclohexyl acetate

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

InchiKey: MBZRJSQZCBXRGK-UHFFFAOYSA-N

Formula: C12H22O2

SMILES: CC(=O)OC1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 198.30

CAS: 1900-69-2

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	1322.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1628.00		NIST Webbook
tb	561.90	K	Joback Method
tc	773.24	K	Joback Method
tf	302.72	K	Joback Method
vc	0.652	m3/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=C1900692&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume