

2-tert-butylcyclohexyl acetate 1

Inchi:	InChI=1S/C12H22O2/c1-9(13)14-11-8-6-5-7-10(11)12(2,3)4/h10-11H,5-8H2,1-4H3
InchiKey:	FINOAUDUYKVGDS-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CC(=O)OC1CCCCC1C(C)(C)C
Mol. weight [g/mol]:	198.30

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
rinsol	1281.60		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/molxK	561.90	Joback Method
cpg	478.84	J/molxK	597.12	Joback Method
cpg	498.39	J/molxK	632.35	Joback Method
cpg	516.77	J/molxK	667.57	Joback Method
cpg	534.02	J/molxK	702.79	Joback Method
cpg	550.18	J/molxK	738.01	Joback Method
cpg	565.28	J/molxK	773.24	Joback Method
dvisc	0.0039043	Paxs	302.72	Joback Method
dvisc	0.0017642	Paxs	345.92	Joback Method

dvisc	0.0009509	Paxs	389.11	Joback Method
dvisc	0.0005799	Paxs	432.31	Joback Method
dvisc	0.0003869	Paxs	475.51	Joback Method
dvisc	0.0002762	Paxs	518.70	Joback Method
dvisc	0.0002076	Paxs	561.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R185187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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