

Ketone, 4-tert-butylcyclohexyl methyl, trans-

Inchi:	InChI=1S/C12H22O/c1-9(13)10-5-7-11(8-6-10)12(2,3)4/h10-11H,5-8H2,1-4H3/t10-,11-
InchiKey:	YMGRIFHYJBXCDV-XYPYZODXSA-N
Formula:	C12H22O
SMILES:	CC(=O)C1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]:	182.30
CAS:	15619-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-59.18	kJ/mol	Joback Method
hf	-378.36	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.428		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	539.48	K	Joback Method
tc	753.13	K	Joback Method
tf	280.49	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.18	J/molxK	539.48	Joback Method
cpg	450.57	J/molxK	575.09	Joback Method
cpg	470.69	J/molxK	610.70	Joback Method
cpg	489.58	J/molxK	646.30	Joback Method
cpg	507.29	J/molxK	681.91	Joback Method
cpg	523.86	J/molxK	717.52	Joback Method
cpg	539.34	J/molxK	753.13	Joback Method
dvisc	0.0056569	Paxs	280.49	Joback Method
dvisc	0.0023995	Paxs	323.66	Joback Method

dvisc	0.0012454	Paxs	366.82	Joback Method
dvisc	0.0007422	Paxs	409.99	Joback Method
dvisc	0.0004881	Paxs	453.15	Joback Method
dvisc	0.0003453	Paxs	496.31	Joback Method
dvisc	0.0002582	Paxs	539.48	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=C15619100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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