cis-4-Tert-butylcyclohexyl methyl ketone

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-PHIMTYICSA-N
Formula: C12H22O
SMILES: CC(=O)C1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 182.30
CAS: 15619-11-1

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/mol×K	539.48	Joback Method
cpg	523.86	J/mol×K	717.52	Joback Method
cpg	507.29	J/mol×K	681.91	Joback Method
cpg	489.58	J/mol×K	646.30	Joback Method
cpg	470.69	J/mol×K	610.70	Joback Method
cpg	450.57	J/mol×K	575.09	Joback Method
cpg	539.34	J/mol×K	753.13	Joback Method
dvisc	0.0002582	Pa×s	539.48	Joback Method
dvisc	0.0003453	Pa×s	496.31	Joback Method

dvisc	0.0004881	Pa×s	453.15	Joback Method
dvisc	0.0007422	Pa×s	409.99	Joback Method
dvisc	0.0012454	Pa×s	366.82	Joback Method
dvisc	0.0023995	Pa×s	323.66	Joback Method
dvisc	0.0056569	Pa×s	280.49	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=C15619111&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume