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
af	0.3774		Cheméo Relay (1.0)
hf	-338.37	kJ/mol	Cheméo Relay (1.0)
hfus	13.93	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
logp	3.428		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	514.96	K	Cheméo Relay (1.0)
tc	728.67	K	Cheméo Relay (1.0)
tf	317.72	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-8.48000e+01
Coeff. B	1.33728e+00
Coeff. C	-8.07700e-04
Coeff. D	1.75860e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.16053e+01
Coeff. B	1.80367e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	280.49
Temperature range (K), max.	527.39

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15619100&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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

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