2-tert-Butylcyclohexanone

Other names: 2-t-Butylcyclohexanone
Cyclohexanone, 2-(1,1-dimethylethyl)-
Inchi: InChI=1S/C10H18O/c1-10(2,3)8-6-4-5-7-9(8)11/h8H,4-7H2,1-3H3
InchiKey: ZRYDPLOWJSFQAE-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC(C)(C)C1CCCCC1=O
Mol. weight [g/mol]: 154.25
CAS: 1728-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-61.98	kJ/mol	Joback Method
hf	-341.86	kJ/mol	Joback Method
hfus	5.59	kJ/mol	Joback Method
hvap	41.23	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	512.34	K	Joback Method
tc	740.09	K	Joback Method
tf	280.48	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.04	J/mol×K	512.34	Joback Method
cpg	361.38	J/mol×K	550.30	Joback Method
cpg	380.56	J/mol×K	588.26	Joback Method
cpg	398.61	J/mol×K	626.21	Joback Method
cpg	415.55	J/mol×K	664.17	Joback Method
cpg	431.39	J/mol×K	702.13	Joback Method
cpg	446.18	J/mol×K	740.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38300e+01
Coeff. B	-3.83144e+03
Coeff. C	-7.48620e+01
Temperature range (K), min.	357.78
Temperature range (K), max.	524.64

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1728467&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume