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
hf	-317.68	kJ/mol	Cheméo Relay (1.0)
hfus	5.59	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
tb	489.95	K	Cheméo Relay (1.0)
tc	709.09	K	Cheméo Relay (1.0)
tf	334.13	K	Cheméo Relay (1.0)

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	0.50	NIST Webbook

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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1728467&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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