

1-t-Butyl-2-hexanone

Other names:	2,2-dimethyl-4-octanone
Inchi:	InChI=1S/C10H20O/c1-5-6-7-9(11)8-10(2,3)4/h5-8H2,1-4H3
InchiKey:	JAODHAABODLKEG-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCC(=O)CC(C)(C)C
Mol. weight [g/mol]:	156.27
CAS:	22319-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-92.76	kJ/mol	Joback Method
hf	-371.06	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	43.30	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
tb	478.84	K	Joback Method
tc	662.03	K	Joback Method
tf	254.81	K	Joback Method
vc	0.591	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.63	J/molxK	478.84	Joback Method
cpg	360.24	J/molxK	509.37	Joback Method
cpg	375.08	J/molxK	539.90	Joback Method
cpg	389.19	J/molxK	570.43	Joback Method
cpg	402.58	J/molxK	600.97	Joback Method
cpg	415.29	J/molxK	631.50	Joback Method
cpg	427.35	J/molxK	662.03	Joback Method
dvisc	0.0064632	Paxs	254.81	Joback Method

dvisc	0.0027020	Paxs	292.15	Joback Method
dvisc	0.0013765	Paxs	329.49	Joback Method
dvisc	0.0008044	Paxs	366.82	Joback Method
dvisc	0.0005192	Paxs	404.16	Joback Method
dvisc	0.0003608	Paxs	441.50	Joback Method
dvisc	0.0002654	Paxs	478.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22319524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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