

t-Butyl isobutyl ketone

Inchi:	InChI=1S/C9H18O/c1-7(2)6-8(10)9(3,4)5/h7H,6H2,1-5H3
InchiKey:	LXFHNTKYSUCXRB-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CC(C)CC(=O)C(C)(C)C
Mol. weight [g/mol]:	142.24
CAS:	14705-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-103.62	kJ/mol	Joback Method
hf	-355.70	kJ/mol	Joback Method
hfus	9.73	kJ/mol	Joback Method
hvap	40.69	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	431.20 ± 3.00	K	NIST Webbook
tb	428.00 ± 3.00	K	NIST Webbook
tb	431.00 ± 4.00	K	NIST Webbook
tb	429.00 ± 3.00	K	NIST Webbook
tc	644.68	K	Joback Method
tf	228.54	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/mol×K	455.52	Joback Method
cpg	315.46	J/mol×K	487.05	Joback Method
cpg	329.87	J/mol×K	518.57	Joback Method
cpg	343.53	J/mol×K	550.10	Joback Method
cpg	356.47	J/mol×K	581.63	Joback Method
cpg	368.73	J/mol×K	613.15	Joback Method

cpg	380.33	J/mol×K	644.68	Joback Method
dvisc	0.0107502	Pa×s	228.54	Joback Method
dvisc	0.0037789	Pa×s	266.37	Joback Method
dvisc	0.0017228	Pa×s	304.20	Joback Method
dvisc	0.0009345	Pa×s	342.03	Joback Method
dvisc	0.0005726	Pa×s	379.86	Joback Method
dvisc	0.0003834	Pa×s	417.69	Joback Method
dvisc	0.0002744	Pa×s	455.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14705501&Units=SI
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
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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