3-Heptanone, 2,4-dimethyl-

Other names: 2,4-Dimethyl-3-heptanone
3-Heptanone, 2,4-Dime
Inchi: InChI=1S/C9H18O/c1-5-6-8(4)9(10)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: MMEXTUAHJZOQKN-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCC(C)C(=O)C(C)C
Mol. weight [g/mol]: 142.24
CAS: 18641-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-108.90	kJ/mol	Joback Method
hf	-352.23	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	41.60	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
ripol	1456.00		NIST Webbook
tb	458.31	K	Joback Method
tc	640.10	K	Joback Method
tf	211.12	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.92	J/mol×K	458.31	Joback Method
cpg	312.19	J/mol×K	488.61	Joback Method
cpg	325.86	J/mol×K	518.91	Joback Method
cpg	338.94	J/mol×K	549.20	Joback Method
cpg	351.45	J/mol×K	579.50	Joback Method
cpg	363.40	J/mol×K	609.80	Joback Method

cpg	374.81	J/mol×K	640.10	Joback Method
dvisc	0.0112700	Pa×s	211.12	Joback Method
dvisc	0.0035885	Pa×s	252.32	Joback Method
dvisc	0.0015755	Pa×s	293.52	Joback Method
dvisc	0.0008471	Pa×s	334.72	Joback Method
dvisc	0.0005218	Pa×s	375.91	Joback Method
dvisc	0.0003537	Pa×s	417.11	Joback Method
dvisc	0.0002572	Pa×s	458.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18641719&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.