2,2-Dimethyl-3-heptanone

Inchi: InChI=1S/C9H18O/c1-5-6-7-8(10)9(2,3)4/h5-7H2,1-4H3
InchiKey: ZLMHETMAEHQFHK-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCC(=O)C(C)(C)C
Mol. weight [g/mol]: 142.24
CAS: 19078-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-101.18	kJ/mol	Joback Method
hf	-350.42	kJ/mol	Joback Method
hfus	13.25	kJ/mol	Joback Method
hvap	41.08	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	964.70		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	965.00		NIST Webbook
tb	441.00 ± 4.00	K	NIST Webbook
tc	640.95	K	Joback Method
tf	243.54	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.18	J/mol×K	455.96	Joback Method
cpg	366.96	J/mol×K	610.12	Joback Method

cpg	354.96	J/mol×K	579.29	Joback Method
cpg	342.31	J/mol×K	548.46	Joback Method
cpg	328.99	J/mol×K	517.62	Joback Method
cpg	314.95	J/mol×K	486.79	Joback Method
cpg	378.33	J/mol×K	640.95	Joback Method
dvisc	0.0002877	Pa×s	455.96	Joback Method
dvisc	0.0003898	Pa×s	420.56	Joback Method
dvisc	0.0005584	Pa×s	385.15	Joback Method
dvisc	0.0008603	Pa×s	349.75	Joback Method
dvisc	0.0014610	Pa×s	314.35	Joback Method
dvisc	0.0028381	Pa×s	278.94	Joback Method
dvisc	0.0066874	Pa×s	243.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19078978&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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume