2-Methyl-5-nonanone

Inchi: InChI=1S/C10H20O/c1-4-5-6-10(11)8-7-9(2)3/h9H,4-8H2,1-3H3
InchiKey: YITHWSJQOVKDGI-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCCCC(=O)CCC(C)C
Mol. weight [g/mol]: 156.27
CAS: 22287-02-1

Physical Properties

Property code	Value	Unit	Source
af	0.5110		Cheméo Relay (1.0)
gf	-98.04	kJ/mol	Joback Method
hf	-387.46	kJ/mol	Cheméo Relay (1.0)
hfus	19.73	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	462.90	K	Cheméo Relay (1.0)
tc	636.21	K	Cheméo Relay (1.0)
tf	257.81	K	Cheméo Relay (1.0)
vc	0.564	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.14	J/mol×K	481.63	Joback Method
cpg	356.94	J/mol×K	511.03	Joback Method
cpg	371.13	J/mol×K	540.42	Joback Method
cpg	384.72	J/mol×K	569.82	Joback Method
cpg	397.72	J/mol×K	599.22	Joback Method
cpg	410.16	J/mol×K	628.61	Joback Method
cpg	422.05	J/mol×K	658.01	Joback Method

dvisc	0.0067728	Pa×s	237.39	Joback Method
dvisc	0.0026268	Pa×s	278.10	Joback Method
dvisc	0.0012976	Pa×s	318.80	Joback Method
dvisc	0.0007520	Pa×s	359.51	Joback Method
dvisc	0.0004869	Pa×s	400.22	Joback Method
dvisc	0.0003417	Pa×s	440.92	Joback Method
dvisc	0.0002545	Pa×s	481.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50947e+01
Coeff. B	-4.22242e+03
Coeff. C	-7.36590e+01
Temperature range (K), min.	358.82
Temperature range (K), max.	505.26

Sources

Cheméo Relay (1.0):

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=C22287021&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

Legend

af: Acentric Factor

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