2,6-Dimethyl-3-heptanone

Other names: 2,6-dimethylheptan-3-one
Inchi: InChI=1S/C9H18O/c1-7(2)5-6-9(10)8(3)4/h7-8H,5-6H2,1-4H3
InchiKey: HFNWDYQEGABWQS-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CC(C)CCC(=O)C(C)C
Mol. weight [g/mol]: 142.24
CAS: 19549-83-8

Physical Properties

Property code	Value	Unit	Source
hf	-359.95	kJ/mol	Cheméo Relay (1.0)
hfus	13.62	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	445.00 ± 4.00	K	NIST Webbook
tf	249.64	K	Cheméo Relay (1.0)

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50525e+01
Coeff. B	-3.96644e+03
Coeff. C	-6.48600e+01
Temperature range (K), min.	333.50
Temperature range (K), max.	472.05

Sources

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

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=C19549838&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point