4,4-Dimethyl-3-hexanone

Inchi: InChI=1S/C8H16O/c1-5-7(9)8(3,4)6-2/h5-6H2,1-4H3
InchiKey: YEDJXYBDQSVPFJ-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCC(=O)C(C)(C)CC
Mol. weight [g/mol]: 128.21
CAS: 19550-14-2

Physical Properties

Property code	Value	Unit	Source
hf	-335.08	kJ/mol	Cheméo Relay (1.0)
hfus	10.66	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
tb	424.20	K	NIST Webbook
tb	426.65 ± 1.50	K	NIST Webbook
tb	424.00 ± 3.00	K	NIST Webbook
tb	424.20 ± 3.00	K	NIST Webbook
tf	247.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.73	J/mol×K	433.08	Joback Method
cpg	271.54	J/mol×K	464.20	Joback Method
cpg	284.66	J/mol×K	495.32	Joback Method
cpg	297.11	J/mol×K	526.44	Joback Method
cpg	308.91	J/mol×K	557.56	Joback Method
cpg	320.09	J/mol×K	588.68	Joback Method
cpg	330.68	J/mol×K	619.80	Joback Method
dvisc	0.0068051	Pa×s	232.27	Joback Method
dvisc	0.0029357	Pa×s	265.74	Joback Method
dvisc	0.0015286	Pa×s	299.21	Joback Method

dvisc	0.0009076	Pa×s	332.67	Joback Method
dvisc	0.0005927	Pa×s	366.14	Joback Method
dvisc	0.0004158	Pa×s	399.61	Joback Method
dvisc	0.0003081	Pa×s	433.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47248e+01
Coeff. B	-3.69868e+03
Coeff. C	-5.82300e+01
Temperature range (K), min.	314.42
Temperature range (K), max.	451.15

Sources

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=C19550142&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

Cheméo Relay (1.0):

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

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point