5-methyl-2-octanone

Inchi: InChI=1S/C9H18O/c1-4-5-8(2)6-7-9(3)10/h8H,4-7H2,1-3H3
InchiKey: UPVLGOPSYZTLGB-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCC(C)CCC(C)=O
Mol. weight [g/mol]: 142.24
CAS: 58654-67-4

Physical Properties

Property code	Value	Unit	Source
af	0.4740		Cheméo Relay (1.0)
gf	-106.46	kJ/mol	Joback Method
hf	-362.15	kJ/mol	Cheméo Relay (1.0)
hfus	17.14	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
tb	459.32	K	Cheméo Relay (1.0)
tc	632.36	K	Cheméo Relay (1.0)
tf	218.25	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.82	J/mol×K	458.75	Joback Method
cpg	372.87	J/mol×K	636.64	Joback Method
cpg	361.70	J/mol×K	606.99	Joback Method
cpg	350.00	J/mol×K	577.34	Joback Method
cpg	337.78	J/mol×K	547.69	Joback Method
cpg	325.02	J/mol×K	518.05	Joback Method
cpg	311.71	J/mol×K	488.40	Joback Method

dvisc	0.0007850	Pa×s	342.44	Joback Method
dvisc	0.0002699	Pa×s	458.75	Joback Method
dvisc	0.0003608	Pa×s	419.98	Joback Method
dvisc	0.0005116	Pa×s	381.21	Joback Method
dvisc	0.0068479	Pa×s	226.12	Joback Method
dvisc	0.0013439	Pa×s	303.66	Joback Method
dvisc	0.0026929	Pa×s	264.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46970e+01
Coeff. B	-3.93944e+03
Coeff. C	-6.71260e+01
Temperature range (K), min.	340.52
Temperature range (K), max.	486.86

Sources

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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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