3-Methyl-4-octanone

Inchi: InChI=1S/C9H18O/c1-4-6-7-9(10)8(3)5-2/h8H,4-7H2,1-3H3
InchiKey: NXTOCVYXABBSGX-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCC(=O)C(C)CC
Mol. weight [g/mol]: 142.24
CAS: 20754-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-106.46	kJ/mol	Joback Method
hf	-346.95	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	41.99	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	447.00 ± 4.00	K	NIST Webbook
tc	636.64	K	Joback Method
tf	226.12	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

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

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50698e+01
Coeff. B	-3.98769e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	335.22
Temperature range (K), max.	474.10

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20754045&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume