6-Methyloctanal

Other names: Octanal, 6-methyl-
Inchi: InChI=1S/C9H18O/c1-3-9(2)7-5-4-6-8-10/h8-9H,3-7H2,1-2H3
InchiKey: ANZKSSJWPUCGOP-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCC(C)CCCCC=O
Mol. weight [g/mol]: 142.24
CAS: 30689-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-77.06	kJ/mol	Joback Method
hf	-319.95	kJ/mol	Joback Method
hfus	17.83	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1058.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1357.00		NIST Webbook
tb	453.54	K	Joback Method
tc	626.89	K	Joback Method
tf	218.19	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.73	J/mol×K	453.54	Joback Method
cpg	361.03	J/mol×K	598.00	Joback Method
cpg	349.61	J/mol×K	569.11	Joback Method
cpg	337.68	J/mol×K	540.22	Joback Method
cpg	325.23	J/mol×K	511.32	Joback Method

cpg	312.25	J/mol×K	482.43	Joback Method
cpg	371.96	J/mol×K	626.89	Joback Method
dvisc	0.0002909	Pa×s	453.54	Joback Method
dvisc	0.0003888	Pa×s	414.31	Joback Method
dvisc	0.0005519	Pa×s	375.09	Joback Method
dvisc	0.0008503	Pa×s	335.87	Joback Method
dvisc	0.0014688	Pa×s	296.64	Joback Method
dvisc	0.0029971	Pa×s	257.42	Joback Method
dvisc	0.0079029	Pa×s	218.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50903e+01
Coeff. B	-4.13479e+03
Coeff. C	-6.81540e+01
Temperature range (K), min.	347.48
Temperature range (K), max.	490.98

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=C30689759&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume