4-nonenal

Inchi: InChI=1S/C9H16O/c1-2-3-4-5-6-7-8-9-10/h5-6,9H,2-4,7-8H2,1H3/b6-5+
InchiKey: QPULDJYQYDGZEI-AATRIKPKSA-N
Formula: C9H16O
SMILES: CCCCC=CCCC=O
Mol. weight [g/mol]: 140.22
CAS: 37423-42-0

Physical Properties

Property code	Value	Unit	Source
gf	5.60	kJ/mol	Joback Method
hf	-197.45	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1096.00		NIST Webbook
tb	458.14	K	Joback Method
tc	635.79	K	Joback Method
tf	228.11	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.56	J/mol×K	458.14	Joback Method
cpg	295.43	J/mol×K	487.75	Joback Method
cpg	307.72	J/mol×K	517.36	Joback Method
cpg	319.44	J/mol×K	546.97	Joback Method
cpg	330.61	J/mol×K	576.57	Joback Method
cpg	341.26	J/mol×K	606.18	Joback Method
cpg	351.41	J/mol×K	635.79	Joback Method
dvisc	0.0047317	Pa×s	228.11	Joback Method

dvisc	0.0020491	Pa×s	266.45	Joback Method
dvisc	0.0010953	Pa×s	304.79	Joback Method
dvisc	0.0006735	Pa×s	343.12	Joback Method
dvisc	0.0004566	Pa×s	381.46	Joback Method
dvisc	0.0003323	Pa×s	419.80	Joback Method
dvisc	0.0002551	Pa×s	458.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47150e+01
Coeff. B	-4.10316e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	357.92
Temperature range (K), max.	509.86

Sources

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

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

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=C37423420&Units=SI

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume