

8-METHYLNONANAL

Inchi:	InChI=1S/C10H20O/c1-10(2)8-6-4-3-5-7-9-11/h9-10H,3-8H2,1-2H3
InchiKey:	WDMOXLRWVGEXJV-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(C)CCCCCCC=O
Mol. weight [g/mol]:	156.27
CAS:	1321-89-7

Physical Properties

Property code	Value	Unit	Source
gf	-68.64	kJ/mol	Joback Method
hf	-340.59	kJ/mol	Joback Method
hfus	20.42	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1171.00		NIST Webbook
ripol	1449.00		NIST Webbook
tb	476.42	K	Joback Method
tc	648.48	K	Joback Method
tf	229.46	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.77	J/molxK	476.42	Joback Method
cpg	357.21	J/molxK	505.10	Joback Method
cpg	371.06	J/molxK	533.77	Joback Method
cpg	384.34	J/molxK	562.45	Joback Method
cpg	397.06	J/molxK	591.13	Joback Method
cpg	409.23	J/molxK	619.81	Joback Method
cpg	420.88	J/molxK	648.48	Joback Method

dvisc	0.0078468	Paxs	229.46	Joback Method
dvisc	0.0029372	Paxs	270.62	Joback Method
dvisc	0.0014251	Paxs	311.78	Joback Method
dvisc	0.0008185	Paxs	352.94	Joback Method
dvisc	0.0005278	Paxs	394.10	Joback Method
dvisc	0.0003698	Paxs	435.26	Joback Method
dvisc	0.0002756	Paxs	476.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50403e+01
Coeff. B	-4.27329e+03
Coeff. C	-7.36590e+01
Temperature range (K), min.	363.32
Temperature range (K), max.	512.90

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback 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=R513829&Units=SI>

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
mccvol:	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

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