

3-Nonanol, 3-methyl-

Other names:	3-Methyl-3-nonanol 3-Methylnonanol-3 3-methylnonan-3-ol
Inchi:	InChI=1S/C10H22O/c1-4-6-7-8-9-10(3,11)5-2/h11H,4-9H2,1-3H3
InchiKey:	VZBFPIMCUSPDLS-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCCC(C)(O)CC
Mol. weight [g/mol]:	158.28
CAS:	21078-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-100.66	kJ/mol	Joback Method
hf	-410.71	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.118		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	517.15	K	Joback Method
tc	683.80	K	Joback Method
tf	265.70	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/molxK	517.15	Joback Method
cpg	447.81	J/molxK	656.02	Joback Method
cpg	436.13	J/molxK	628.25	Joback Method
cpg	423.89	J/molxK	600.47	Joback Method
cpg	411.07	J/molxK	572.70	Joback Method
cpg	397.63	J/molxK	544.92	Joback Method

cpg	458.94	J/molxK	683.80	Joback Method
dvisc	0.0001201	Paxs	517.15	Joback Method
dvisc	0.0002077	Paxs	475.24	Joback Method
dvisc	0.0003993	Paxs	433.33	Joback Method
dvisc	0.0008829	Paxs	391.43	Joback Method
dvisc	0.0023619	Paxs	349.52	Joback Method
dvisc	0.0082611	Paxs	307.61	Joback Method
dvisc	0.0428890	Paxs	265.70	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.59232e+01
Coeff. B	-4.65086e+03
Coeff. C	-7.51460e+01
Temperature range (K), min.	372.60
Temperature range (K), max.	513.42

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

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

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C21078728&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
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

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