

4-Nonanol, 4-methyl-

Other names:	4-Methyl-4-nonanol 4-methylnonan-4-ol
Inchi:	InChI=1S/C10H22O/c1-4-6-7-9-10(3,11)8-5-2/h11H,4-9H2,1-3H3
InchiKey:	GDCOAKPWVJCNGI-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCC(C)(O)CCC
Mol. weight [g/mol]:	158.28
CAS:	23418-38-4

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/mol×K	517.15	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method
cpg	458.94	J/mol×K	683.80	Joback Method

dvisc	0.0428890	Pa×s	265.70	Joback Method
dvisc	0.0082611	Pa×s	307.61	Joback Method
dvisc	0.0023619	Pa×s	349.52	Joback Method
dvisc	0.0008829	Pa×s	391.43	Joback Method
dvisc	0.0003993	Pa×s	433.33	Joback Method
dvisc	0.0002077	Pa×s	475.24	Joback Method
dvisc	0.0001201	Pa×s	517.15	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:	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
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=C23418384&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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