3-Nonanol, 2-methyl-

Other names: 2-Methyl-3-nonanol
Inchi: InChI=1S/C10H22O/c1-4-5-6-7-8-10(11)9(2)3/h9-11H,4-8H2,1-3H3
InchiKey: OFIYMUXECPHIPZ-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCCC(O)C(C)C
Mol. weight [g/mol]: 158.28
CAS: 26533-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	481.55 ± 1.00	K	NIST Webbook
tb	473.15 ± 4.00	K	NIST Webbook
tc	683.75	K	Joback Method
tf	233.28	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/mol×K	519.50	Joback Method
cpg	394.90	J/mol×K	546.87	Joback Method
cpg	408.18	J/mol×K	574.25	Joback Method
cpg	420.93	J/mol×K	601.62	Joback Method
cpg	433.16	J/mol×K	629.00	Joback Method
cpg	444.88	J/mol×K	656.37	Joback Method
cpg	456.11	J/mol×K	683.75	Joback Method

dvisc	0.1480969	Pa×s	233.28	Joback Method
dvisc	0.0161218	Pa×s	280.98	Joback Method
dvisc	0.0033408	Pa×s	328.69	Joback Method
dvisc	0.0010317	Pa×s	376.39	Joback Method
dvisc	0.0004150	Pa×s	424.09	Joback Method
dvisc	0.0002007	Pa×s	471.80	Joback Method
dvisc	0.0001109	Pa×s	519.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63938e+01
Coeff. B	-4.78707e+03
Coeff. C	-7.50210e+01
Temperature range (K), min.	372.24
Temperature range (K), max.	506.98

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=C26533335&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume