

4-Nonanol, 2,6,8-trimethyl-

Other names:	2,4,8-Trimethyl-6-nonanol 2,6,8-Trimethyl-4-nonanol 2,6,8-Trimethylnonanol-4 2,6,8-trimethylnonan-4-ol 4-Hydroxy-2,6,8-trimethylnonane
Inchi:	InChI=1S/C12H26O/c1-9(2)6-11(5)8-12(13)7-10(3)4/h9-13H,6-8H2,1-5H3
InchiKey:	LFEHSRSSAGQWNI-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CC(C)CC(C)CC(O)CC(C)C
Mol. weight [g/mol]:	186.33
CAS:	123-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.42	kJ/mol	Joback Method
hf	-464.36	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.466		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
tb	498.55	K	NIST Webbook
tb	498.65	K	NIST Webbook
tc	732.65	K	Joback Method
tf	225.82	K	Joback Method
vc	0.703	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.59	J/mol×K	564.38	Joback Method
cpg	495.41	J/mol×K	592.43	Joback Method
cpg	510.55	J/mol×K	620.47	Joback Method

cpg	525.05	J/molxK	648.52	Joback Method
cpg	538.91	J/molxK	676.56	Joback Method
cpg	552.17	J/molxK	704.61	Joback Method
cpg	564.82	J/molxK	732.65	Joback Method
dvisc	0.4438389	Paxs	225.82	Joback Method
dvisc	0.0236653	Paxs	282.25	Joback Method
dvisc	0.0033514	Paxs	338.67	Joback Method
dvisc	0.0008295	Paxs	395.10	Joback Method
dvisc	0.0002910	Paxs	451.53	Joback Method
dvisc	0.0001289	Paxs	507.95	Joback Method
dvisc	0.0000672	Paxs	564.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64058e+01
Coeff. B	-4.93242e+03
Coeff. C	-7.97050e+01
Temperature range (K), min.	385.72
Temperature range (K), max.	524.29

Sources

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=C123171&Units=SI
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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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