4-Heptanol, 2,6-dimethyl-

Other names:	2,6-Dimethyl-4-heptanol
	2,6-Dimethylheptanol-4
	2,6-dimethylheptan-4-ol
	DIISOBUTYLCARBINOL
	NONYL ALCOHOL
	SEC-NONYL ALCOHOL
	diisobutyl carbinol
Inchi:	InChI=1S/C9H20O/c1-7(2)5-9(10)6-8(3)4/h7-10H,5-6H2,1-4H3
InchiKey:	HXQPUEQDBSPXTE-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CC(C)CC(O)CC(C)C
Mol. weight [g/mol]:	144.25
CAS:	108-82-7

Physical Properties

Property code	Value	Unit	Source
gf	-119.24	kJ/mol	Joback Method
hf	-397.16	kJ/mol	Joback Method
hfus	12.58	kJ/mol	Joback Method
hvap	65.20 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.440		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
ripol	1480.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1509.00		NIST Webbook
tb	496.18	K	Joback Method
tc	664.60	K	Joback Method
tf	207.01	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.97	J/mol×K	496.18	Joback Method
cpg	348.32	J/mol×K	524.25	Joback Method
cpg	361.14	J/mol×K	552.32	Joback Method
cpg	373.44	J/mol×K	580.39	Joback Method
cpg	385.22	J/mol×K	608.46	Joback Method
cpg	396.50	J/mol×K	636.53	Joback Method
cpg	407.30	J/mol×K	664.60	Joback Method
dvisc	0.5757064	Pa×s	207.01	Joback Method
dvisc	0.0376026	Pa×s	255.20	Joback Method
dvisc	0.0058439	Pa×s	303.40	Joback Method
dvisc	0.0015130	Pa×s	351.59	Joback Method
dvisc	0.0005426	Pa×s	399.79	Joback Method
dvisc	0.0002426	Pa×s	447.98	Joback Method
dvisc	0.0001269	Pa×s	496.18	Joback Method
hvapt	54.50	kJ/mol	408.00	NIST Webbook
hvapt	52.80	kJ/mol	413.00	NIST Webbook
pvap	4.91e-03	kPa	278.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	7.90e-03	kPa	283.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.01	kPa	288.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.02	kPa	291.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.02	kPa	294.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.03	kPa	297.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.04	kPa	300.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.05	kPa	303.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.06	kPa	306.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.10	kPa	312.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

pvap	0.13	kPa	315.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.17	kPa	318.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.21	kPa	321.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65373e+01
Coeff. B	-4.57057e+03
Coeff. C	-6.65280e+01
Temperature range (K), min.	347.80
Temperature range (K), max.	473.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.19840e+02
Coeff. B	-1.17511e+04
Coeff. C	-1.47552e+01
Coeff. D	5.20216e-06
Temperature range (K), min.	208.00
Temperature range (K), max.	603.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108827&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol848.mol
Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols:	https://www.doi.org/10.1021/je049561m
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=848
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume