

3-Heptanol, 3,6-dimethyl-

Other names:	3,6-Dimethyl-3-heptanol
Inchi:	InChI=1S/C9H20O/c1-5-9(4,10)7-6-8(2)3/h8,10H,5-7H2,1-4H3
InchiKey:	HVPGGLNDHUWMLS-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCC(C)(O)CCC(C)C
Mol. weight [g/mol]:	144.25
CAS:	1573-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-111.52	kJ/mol	Joback Method
hf	-395.35	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	50.62	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	987.00		NIST Webbook
tb	446.15 ± 2.00	K	NIST Webbook
tc	664.90	K	Joback Method
tf	239.43	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.46	J/molxK	493.83	Joback Method
cpg	399.69	J/molxK	636.39	Joback Method
cpg	388.42	J/molxK	607.88	Joback Method
cpg	376.59	J/molxK	579.36	Joback Method
cpg	364.17	J/molxK	550.85	Joback Method
cpg	351.13	J/molxK	522.34	Joback Method

cpg	410.41	J/molxK	664.90	Joback Method
dvisc	0.0001397	Paxs	493.83	Joback Method
dvisc	0.0002546	Paxs	451.43	Joback Method
dvisc	0.0005256	Paxs	409.03	Joback Method
dvisc	0.0012828	Paxs	366.63	Joback Method
dvisc	0.0039538	Paxs	324.23	Joback Method
dvisc	0.0170986	Paxs	281.83	Joback Method
dvisc	0.1242076	Paxs	239.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64265e+01
Coeff. B	-4.49856e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	343.92
Temperature range (K), max.	469.91

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1573280&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/ci9903071
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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