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/mol×K	493.83	Joback Method
cpg	399.69	J/mol×K	636.39	Joback Method
cpg	388.42	J/mol×K	607.88	Joback Method
cpg	376.59	J/mol×K	579.36	Joback Method
cpg	364.17	J/mol×K	550.85	Joback Method
cpg	351.13	J/mol×K	522.34	Joback Method

cpg	410.41	J/mol×K	664.90	Joback Method
dvisc	0.0001397	Pa×s	493.83	Joback Method
dvisc	0.0002546	Pa×s	451.43	Joback Method
dvisc	0.0005256	Pa×s	409.03	Joback Method
dvisc	0.0012828	Pa×s	366.63	Joback Method
dvisc	0.0039538	Pa×s	324.23	Joback Method
dvisc	0.0170986	Pa×s	281.83	Joback Method
dvisc	0.1242076	Pa×s	239.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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=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/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
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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