3-Heptanol, 2,6-dimethyl-

Other names: 2,6-Dimethyl-3-heptanol
Inchi: InChI=1S/C9H20O/c1-7(2)5-6-9(10)8(3)4/h7-10H,5-6H2,1-4H3
InchiKey: XZDMJRIWJSNEGC-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CC(C)CCC(O)C(C)C
Mol. weight [g/mol]: 144.25
CAS: 19549-73-6

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	51.14	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.440		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
tb	444.15 ± 5.00	K	NIST Webbook
tb	448.15 ± 5.00	K	NIST Webbook
tb	448.65 ± 4.00	K	NIST Webbook
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69034e+01
Coeff. B	-4.64883e+03
Coeff. C	-6.57360e+01
Temperature range (K), min.	345.52
Temperature range (K), max.	466.78

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549736&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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