

3-Hexanol, 2,5-dimethyl-

Other names:	2,5-Dimethyl-3-hexanol 2,5-dimethylhexan-3-ol
Inchi:	InChI=1S/C8H18O/c1-6(2)5-8(9)7(3)4/h6-9H,5H2,1-4H3
InchiKey:	SNKTZHPOKPYBPT-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)CC(O)C(C)C
Mol. weight [g/mol]:	130.23
CAS:	19550-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-127.66	kJ/mol	Joback Method
hf	-376.52	kJ/mol	Joback Method
hfus	9.99	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.049		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	473.30	K	Joback Method
tc	642.89	K	Joback Method
tf	195.74	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.54	J/mol×K	473.30	Joback Method
cpg	303.02	J/mol×K	501.56	Joback Method
cpg	314.99	J/mol×K	529.83	Joback Method
cpg	326.48	J/mol×K	558.09	Joback Method
cpg	337.49	J/mol×K	586.36	Joback Method
cpg	348.04	J/mol×K	614.62	Joback Method
cpg	358.15	J/mol×K	642.89	Joback Method

dvisc	0.9006667	Paxs	195.74	Joback Method
dvisc	0.0532070	Paxs	242.00	Joback Method
dvisc	0.0077930	Paxs	288.26	Joback Method
dvisc	0.0019417	Paxs	334.52	Joback Method
dvisc	0.0006781	Paxs	380.78	Joback Method
dvisc	0.0002974	Paxs	427.04	Joback Method
dvisc	0.0001533	Paxs	473.30	Joback Method
hvapt	55.00	kJ/mol	384.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58903e+01
Coeff. B	-4.06498e+03
Coeff. C	-7.03730e+01
Temperature range (K), min.	330.90
Temperature range (K), max.	454.63

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550073&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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