1-Hexyn-3-ol, 3,5-dimethyl-

Other names:	3,5-Dimethyl-1-hexyn-3-ol
	3,5-Dimethyl-1-hexyne-3-ol
	3,5-dimethylhex-1-yn-3-ol
	DL-3,5-Dimethyl-1-hexyn-3-ol
	Surfynol
	Surfynol 61
Inchi:	InChI=1S/C8H14O/c1-5-8(4,9)6-7(2)3/h1,7,9H,6H2,2-4H3
InchiKey:	NECRQCBKTGZNMH-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	C#CC(C)(O)CC(C)C
Mol. weight [g/mol]:	126.20
CAS:	107-54-0

Physical Properties

Property code	Value	Unit	Source
gf	103.13	kJ/mol	Joback Method
hf	-82.81	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	48.25	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.417		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	423.65 ± 3.00	K	NIST Webbook
tb	423.50 ± 0.50	K	NIST Webbook
tb	423.70	K	NIST Webbook
tc	645.04	K	Joback Method
tf	275.13	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.57	J/mol×K	461.07	Joback Method
cpg	273.12	J/mol×K	491.73	Joback Method
cpg	284.04	J/mol×K	522.39	Joback Method
cpg	294.34	J/mol×K	553.06	Joback Method
cpg	304.06	J/mol×K	583.72	Joback Method
cpg	313.24	J/mol×K	614.38	Joback Method
cpg	321.90	J/mol×K	645.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64497e+01
Coeff. B	-4.31563e+03
Coeff. C	-5.89390e+01
Temperature range (K), min.	326.15
Temperature range (K), max.	446.15

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107540&Units=SI

Legend

cpg: Ideal gas heat capacity
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