3-Hexanol, 3-ethyl-

Other names: 1,1-Diethyl-1-butanol
3-Ethyl-3-hexanol
3-ethylhexan-3-ol
Inchi: InChI=1S/C8H18O/c1-4-7-8(9,5-2)6-3/h9H,4-7H2,1-3H3
InchiKey: WNDLTOTUHMHNOC-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCCC(O)(CC)CC
Mol. weight [g/mol]: 130.23
CAS: 597-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-117.50	kJ/mol	Joback Method
hf	-369.43	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	431.65 ± 3.00	K	NIST Webbook
tb	432.15 ± 3.00	K	NIST Webbook
tb	433.25 ± 2.00	K	NIST Webbook
tb	433.15 ± 3.00	K	NIST Webbook
tc	640.25	K	Joback Method
tf	243.16	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.77	J/mol×K	640.25	Joback Method
cpg	292.85	J/mol×K	471.39	Joback Method
cpg	305.37	J/mol×K	499.53	Joback Method

cpg	317.32	J/mol×K	527.68	Joback Method
cpg	328.71	J/mol×K	555.82	Joback Method
cpg	339.57	J/mol×K	583.96	Joback Method
cpg	349.91	J/mol×K	612.10	Joback Method
dvisc	0.0001803	Pa×s	471.39	Joback Method
dvisc	0.0742698	Pa×s	243.16	Joback Method
dvisc	0.0138116	Pa×s	281.20	Joback Method
dvisc	0.0038351	Pa×s	319.24	Joback Method
dvisc	0.0013989	Pa×s	357.27	Joback Method
dvisc	0.0006196	Pa×s	395.31	Joback Method
dvisc	0.0003166	Pa×s	433.35	Joback Method
hvapt	49.20	kJ/mol	382.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60042e+01
Coeff. B	-4.33157e+03
Coeff. C	-5.28160e+01
Temperature range (K), min.	328.42
Temperature range (K), max.	457.91

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=C597762&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
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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