

1-Hexanol, 2,2-dimethyl-

Other names:	2,2-Dimethyl-1-hexanol 2,2-Dimethylhexanol Neooctanol tert-Octanol tert-Octyl alcohol
Inchi:	InChI=1S/C8H18O/c1-4-5-6-8(2,3)7-9/h9H,4-7H2,1-3H3
InchiKey:	GSSDZVRLQDXOPL-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(C)(C)CO
Mol. weight [g/mol]:	130.23
CAS:	2370-13-0

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	-2.19		Crippen Method
logp	2.195		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	440.65 ± 5.00	K	NIST Webbook
tb	445.65 ± 5.00	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	292.85	J/mol×K	471.39	Joback Method
cpg	349.91	J/mol×K	612.10	Joback Method
cpg	339.57	J/mol×K	583.96	Joback Method

cpg	328.71	J/mol×K	555.82	Joback Method
cpg	317.32	J/mol×K	527.68	Joback Method
cpg	305.37	J/mol×K	499.53	Joback Method
cpg	359.77	J/mol×K	640.25	Joback Method
dvisc	0.0001803	Pa×s	471.39	Joback Method
dvisc	0.0003166	Pa×s	433.35	Joback Method
dvisc	0.0006196	Pa×s	395.31	Joback Method
dvisc	0.0013989	Pa×s	357.27	Joback Method
dvisc	0.0038351	Pa×s	319.24	Joback Method
dvisc	0.0138116	Pa×s	281.20	Joback Method
dvisc	0.0742698	Pa×s	243.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	3.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47185e+01
Coeff. B	-3.27106e+03
Coeff. C	-1.21790e+02
Temperature range (K), min.	348.46
Temperature range (K), max.	469.51

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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>

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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