

3-Octanol, 2-methyl-

Other names:	2-Methyl-3-octanol 2-methyloctan-3-ol
Inchi:	InChI=1S/C9H20O/c1-4-5-6-7-9(10)8(2)3/h8-10H,4-7H2,1-3H3
InchiKey:	DIVBBSLQUDHECU-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCC(O)C(C)C
Mol. weight [g/mol]:	144.25
CAS:	26533-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-391.88	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.584		Crippen Method
mvol	143.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1092.00		NIST Webbook
tb	457.15 ± 3.00	K	NIST Webbook
tc	661.81	K	Joback Method
tf	222.01	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.77	J/mol×K	496.62	Joback Method
cpg	347.81	J/mol×K	524.15	Joback Method
cpg	360.33	J/mol×K	551.68	Joback Method
cpg	372.35	J/mol×K	579.21	Joback Method
cpg	383.89	J/mol×K	606.75	Joback Method
cpg	394.96	J/mol×K	634.28	Joback Method

cpg	405.56	J/mol×K	661.81	Joback Method
dvisc	0.2091511	Paxs	222.01	Joback Method
dvisc	0.0215322	Paxs	267.78	Joback Method
dvisc	0.0043049	Paxs	313.55	Joback Method
dvisc	0.0012970	Paxs	359.31	Joback Method
dvisc	0.0005125	Paxs	405.08	Joback Method
dvisc	0.0002445	Paxs	450.85	Joback Method
dvisc	0.0001337	Paxs	496.62	Joback Method
hvapt	49.50	kJ/mol	420.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64159e+01
Coeff. B	-4.58821e+03
Coeff. C	-6.82380e+01
Temperature range (K), min.	352.72
Temperature range (K), max.	481.43

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=C26533346&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/ci9903071

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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