

4-Octanol, 7-methyl-

Other names:	7-Methyl-4-octanol 7-methyloctan-4-ol
Inchi:	InChI=1S/C9H20O/c1-4-5-9(10)7-6-8(2)3/h8-10H,4-7H2,1-3H3
InchiKey:	KJMBBHZOLRRVMV-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCC(O)CCC(C)C
Mol. weight [g/mol]:	144.25
CAS:	33933-77-6

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
mcvol	143.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	496.62	K	Joback Method
tc	661.81	K	Joback Method
tf	222.01	K	Joback Method
vc	0.546	m3/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	Pa×s	222.01	Joback Method
dvisc	0.0215322	Pa×s	267.78	Joback Method
dvisc	0.0043049	Pa×s	313.55	Joback Method
dvisc	0.0012970	Pa×s	359.31	Joback Method
dvisc	0.0005125	Pa×s	405.08	Joback Method
dvisc	0.0002445	Pa×s	450.85	Joback Method
dvisc	0.0001337	Pa×s	496.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52842e+01
Coeff. B	-4.24943e+03
Coeff. C	-6.76400e+01
Temperature range (K), min.	351.00
Temperature range (K), max.	493.75

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33933776&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
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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