

4-Octanol, 2,7-dimethyl-

Other names:	2,7-Dimethyl-4-octanol
Inchi:	InChI=1S/C10H22O/c1-8(2)5-6-10(11)7-9(3)4/h8-11H,5-7H2,1-4H3
InchiKey:	FRJOBNOTOHIMIH-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CC(C)CCC(O)CC(C)C
Mol. weight [g/mol]:	158.28
CAS:	19781-11-4

Physical Properties

Property code	Value	Unit	Source
gf	-110.82	kJ/mol	Joback Method
hf	-417.80	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.830		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	519.06	K	Joback Method
tc	686.37	K	Joback Method
tf	218.28	K	Joback Method
vc	0.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.30	J/molxK	519.06	Joback Method
cpg	395.45	J/molxK	546.94	Joback Method
cpg	409.03	J/molxK	574.83	Joback Method
cpg	422.04	J/molxK	602.71	Joback Method
cpg	434.51	J/molxK	630.60	Joback Method
cpg	446.45	J/molxK	658.48	Joback Method
cpg	457.87	J/molxK	686.37	Joback Method
dvisc	0.3779599	Paxs	218.28	Joback Method

dvisc	0.0269801	Paxs	268.41	Joback Method
dvisc	0.0044205	Paxs	318.54	Joback Method
dvisc	0.0011845	Paxs	368.67	Joback Method
dvisc	0.0004350	Paxs	418.80	Joback Method
dvisc	0.0001979	Paxs	468.93	Joback Method
dvisc	0.0001048	Paxs	519.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52748e+01
Coeff. B	-4.40441e+03
Coeff. C	-7.32420e+01
Temperature range (K), min.	367.12
Temperature range (K), max.	515.30

Sources

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=C19781114&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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