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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0269801	Pa×s	268.41	Joback Method
dvisc	0.0044205	Pa×s	318.54	Joback Method
dvisc	0.0011845	Pa×s	368.67	Joback Method
dvisc	0.0004350	Pa×s	418.80	Joback Method
dvisc	0.0001979	Pa×s	468.93	Joback Method
dvisc	0.0001048	Pa×s	519.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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