5-Nonanol, 5-methyl-

Other names: 2-Butyl-2-hexanol
5-Methyl-5-nonanol
Inchi: InChI=1S/C10H22O/c1-4-6-8-10(3,11)9-7-5-2/h11H,4-9H2,1-3H3
InchiKey: AGSIGVZAVLOKLP-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCC(C)(O)CCCC
Mol. weight [g/mol]: 158.28
CAS: 33933-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-100.66	kJ/mol	Joback Method
hf	-410.71	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.118		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	517.15	K	Joback Method
tc	683.80	K	Joback Method
tf	265.70	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/mol×K	517.15	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	458.94	J/mol×K	683.80	Joback Method

dvisc	0.0001201	Pa×s	517.15	Joback Method
dvisc	0.0002077	Pa×s	475.24	Joback Method
dvisc	0.0003993	Pa×s	433.33	Joback Method
dvisc	0.0008829	Pa×s	391.43	Joback Method
dvisc	0.0023619	Pa×s	349.52	Joback Method
dvisc	0.0082611	Pa×s	307.61	Joback Method
dvisc	0.0428890	Pa×s	265.70	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=C33933787&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